**Université de Montréal**

# Invariant discretizations of partial differential equations

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# RÉSUMÉ

Un algorithme permettant de discrétiser les équations aux dérivées partielles (EDP) tout en préservant leurs symétries de Lie est élaboré. Ceci est rendu possible grâce à l'utilisation de dérivées partielles discrètes se transformant comme les dérivées partielles continues sous l'action de groupes de Lie locaux. Dans les applications, beaucoup d'EDP sont invariantes sous l'action de transformations ponctuelles de Lie de dimension infinie qui font partie de ce que l'on désigne comme des pseudo-groupes de Lie. Afin d'étendre la méthode de discrétisation préservant les symétries à ces équations, une discrétisation des pseudo-groupes est proposée. Cette discrétisation a pour effet de transformer les symétries ponctuelles en symétries généralisées dans l'espace discret. Des schémas invariants sont ensuite créés pour un certain nombre d'EDP. Dans tous les cas, des tests numériques montrent que les schémas invariants approximent mieux leur équivalent continu que les différences finies standard.

**Mots clefs** : équation aux dérivées partielles, pseudo-groupe de Lie, symétrie, schéma invariant, équation aux différences finies, analyse numérique, repère mobile, invariant différentiel.

# SUMMARY

An algorithm discretizing partial differential equations (PDEs) while preserving their Lie symmetries is provided. This is made possible by the use of discrete partial derivatives transforming as their continuous counterparts under the action of local Lie groups. In applications, many PDEs are invariant under the action of Lie point symmetries of infinite dimension designated as Lie pseudo-groups. To extend the invariant discretization method to such equations, a discretization of pseudo-groups is proposed. The pseudo-group action discretization transforms the continuous point symmetries into generalized symmetries in the discrete space. Invariant schemes are then created for a number of PDEs. In all cases, numerical tests demonstrate that invariant schemes are better approximations of their continuous equivalents than standard finite differences.

**Key words**: partial differential equation, Lie pseudo-group, symmetry, invariant scheme, finite difference equation, numerical analysis, moving frame, differential invariant, joint invariant.

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# Chapter 1

## INTRODUCTION

The main goal of this thesis is to develop a method for producing discrete approximations of partial differential equations that “preserve” their symmetries. This process will be referred throughout the thesis as *invariant discretization*. The symmetries considered are continuous transformations which send, for a given system, solutions to solutions. The study of these continuous symmetries of differential equations was pioneered by Lie in the late 19th century and numerous applications have since been found. Symmetries were a cornerstone of mathematical physics during the 20th century. The most well-known and probably most well-illustrated example of symmetry arose in the axioms of Einstein’s relativity when he postulated that the speed of light was invariant under change of inertial frames of reference. Or, in mathematical terms, that the equations describing light “movements” should be invariant under Lorentz transformations. Symmetries then played a crucial role in the standard model developed in particle physics during the second half of the 20th century. In the standard model, each interaction is governed by a continuous symmetry group. Since relativity coupled with the standard model describes the four known forces present in our universe, symmetry principles are inextricably linked to our current understanding of nature.

Symmetry in nature has always amazed observers attentive to its manifestations and drawn the attention of philosophers and scientists. For the poet, it is harmony of a nearly mystical quality found in nature; for the scientist, a means to understand our universe and break down its complexity into simpler fundamental blocks. The concept of symmetry has been present since time immemorial in our quest to understand our surroundings. From Plato arguing that matter was made of microscopic polyhedra or Copernic using circular orbits to describe the planets' movement around the sun, the human mind has always been fascinated by symmetric objects for their beauty and simplicity. As those two examples suggest, scientists have sometimes been a bit too naive and sure about the world's complexity. However, they highlight our on-going and legitimate quest to describe nature with the fewest and most harmonious basic principles. Einstein's relativity and the standard model attest to the fact that identifying symmetries present in nature helps us understand the building blocks of our universe.

Lie's theory was a major step forward providing mathematical tools to encode continuous symmetries into algebra. From the invention of differential calculus in the late 17th century up to the late 19th century, differential equations had become by the end of the 19th century one of the main mathematical tools for describing movement and, more generally, any dynamical process. Lie's theory then made it possible to answer fundamental questions such as: "What are all the continuous symmetries admitted by a given differential equation?" or "If we want to construct a model or a theory respecting certain observed symmetries of a given phenomenon, what differential equations are admissible?" From a practical point of view, Lie's techniques have been a powerful tool for solving differential equations, [**48**]. In fact, most known techniques to solve nonlinear differential equations are derived from Lie's theory.

The applications of Lie's theory to fluid mechanics equations gained in popularity during the mid 20th century thanks to G. Birkhoff, Ovsiannikov and others, [**5, 58**]. More or less during the same period, the first commercial computer was invented and the field of modern numerical analysis, i.e. assisted by computers, slowly began to take shape. In this context, in the early 70s, Yanenko and Shokin considered the possibility of applying the continuous group theory to discrete fluid mechanics equations, [**70**]. However, they were still using a combination of differential and difference equations. The transition to fully discrete equations seem to have slowly germinated during the 80s, in Maeda's work in particular, [**45**]. The quest to recast Lie's theory in a discrete space really started in the early 90s with the simultaneous works of Dorodnitsyn, [**18**], Levi and Winternitz, [**39**]. In 2000, Dorodnitsyn, Kozlov and Winternitz published a classification of second-order ordinary difference equations with respect to their symmetries, [**20**]. It was the discrete equivalent of Lie's famous classification of second order differential equations done a century earlier. The natural progression would be to use those symmetries to find solutions of discrete equations through a process called *symmetry reduction*. However, it turned out that symmetry reduction was not straightforward for discrete equations. They managed to find solutions of discrete equations using a discrete version of Noether's theorem, [**21**], with the drawback that the method could only be applied to equations that were some sort of discrete Euler-Lagrange equations. They recently extended this result to a larger class of equations, [**23**]. All these advances in the discrete world were made using the infinitesimal approach inherited from Lie which uses the algebra instead of the group of symmetry.

In the mean-time, Olver and Fels were working on a different approach for studying invariants of Lie groups inspired by the work of Cartan, [**11**]. The latter, once a student of Lie, developed a more abstract treatment of Lie groups based on differential geometry. In Cartan's approach, differential forms are used instead of infinitesimal generators of the group's algebra. This theory, revisited and reformulated by Fels and Olver, [**26, 27**], has proven to be extremely powerful in various aspects of the application of Lie groups to differential equations. It uses an object called a "moving frame" to generate invariants. A few years later, Olver laid down the groundwork for the application of the moving frame method to ordinary difference equations, [**50**], and, eventually, to partial difference equations, [**53**].

Whether based on the infinitesimal approach used by Dorodnitsyn, Kozlov, Levi and Winternitz or the moving frame method used by Olver and Fels, a number of invariant schemes were found over the years for particular equations, including Burgers' equation, the Schrödinger equation and variations on the heat equation to name only a few. In addition to the authors mentioned previously, Bihlo, Budd, Kim, Quispel, Rodriguez and Valiquette contributed to the theory and are responsible for the computation of a number of examples showing that invariant schemes can produce better results than standard numerical techniques, [**2, 6, 32, 38, 61, 65, 69**]. Many others have contributed to the field during the last twenty-five years and this is by no means an extensive review, but merely a tribute to the works which have influenced me the most on my intellectual path.

From a practical point of view, numerical computations are the main motivation for developing invariant discrete methods since we mostly rely on computers to find solutions for nonlinear differential equations arising in physical models and computers only manipulate discrete data. There are also theoretical motivations to develop

Lie's theory in a discrete space. In quantum mechanics, the Planck length is an unbreakable minimal distance at which objects cannot be moved closer to each other. Although this length is so small that no instrument can yet test this hypothesis, it indicates the possibility of a discrete step separating all things in the universe. Researchers have also been able to eliminate the infinite quantities appearing in quantum field theory by discretizing space, [**17**]. It is an alternative to renormalization procedures. Finally, some physical problems are discrete by nature and, in these cases, it is the differential equations which are continuous approximations of reality.

This thesis structure is as follows. Chapter 2 presents the main theoretical concepts used herewith. Examples are provided to facilitate understanding of the theory and improve the capacity of non-expert readers to smoothly absorb the content presented in the two articles that then follow. The main subjects presented are Lie pseudo-groups, the continuous and discrete spaces they act upon, moving frames as a tool to produce invariants and, finally, the construction of invariant discretizations for PDEs invariant under the action of Lie pseudo-groups.

Chapter 3 consists of the first article presented in this thesis. It develops an invariant discretization method for PDEs using moving frames. The question motivating the research was first evoked by Winternitz and Levi. They were working with Scimiterna and Thomova on an article, [**37**], in which they would write down the prolongation of Lie algebra generators for ordinary difference schemes in terms of discrete derivatives and wondered if the process could be done for partial difference schemes. The main difficulty which had to be dealt with was the fact that, for PDEs, standard finite differences on arbitrary meshes did not converge, in general, to the continuous derivatives they were supposed to approximate. This was problematic since invariant meshes are typically non-uniform and non-orthogonal. Our article proposes a simpler alternative to Olver's approach, [**53**], by using a different definition of partial discrete derivatives. In both cases, discrete partial derivatives are chosen such that they converge toward their continuous counterparts even on arbitrary meshes. By construction, these discrete derivatives converge toward the continuous derivatives even after being acted upon by Lie groups. This, in turn, makes it possible to discretize PDEs invariant under Lie groups while preserving symmetries. The article ends with numerical simulations illustrating that invariant discretizations produce more precise approximations of certain solutions for given differential equations when compared to some standard methods. It is important to note that Olver also proposed a way to apply the theory of moving frames to partial difference schemes, [**53**].

Chapter 4 consists of the second article presented in this thesis. It discusses the invariant discretization of PDEs invariant under Lie pseudo-groups. It was inspired by the recent work of Olver and Pohjanpelto, [**54, 55**], who developed the application of the moving frame theory to Lie infinite dimensional pseudo-groups. Lie pseudo-groups are an infinite dimensional generalization of local Lie group actions. These pseudo-groups arise in a number of applications in physics: gauge symmetries, fluid and plasma mechanics and hydrodynamics to name only a few. To our knowledge, this article presents the first method for producing invariant schemes of PDEs invariant under Lie pseudo-groups. In order to do this, a certain number of concepts of the moving frame theory applied to continuous space were redefined in a discrete space setting. Once this was done, a new object called a *discretized pseudo-group* was defined in order to apply our method of invariant discretization of PDEs. *Discretized pseudo-groups* are discrete approximations of continuous pseudo-groups. The method was then applied to produce an invariant numerical scheme for a differential equation. The invariant scheme was then compared to a standard one for boundary value problems (BVP) on rectangles. Once again, the invariant method proved to be more precise and stable near singularities than the standard one.

Chapter 5 summarizes the main results of the thesis and outlines potential avenues for future research.

# Chapter 2

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## PRELIMINARIES

This chapter focuses on introducing the main objects used in the following articles. The reader should be familiar with the theory of symmetry groups of differential equations. If not, the reader is invited to read the first three chapters of Olver's book *Applications of Lie Groups to Differential Equations*, [**48**].

### 2.1. Lie pseudo-groups

Lie pseudo-groups are an infinite-dimensional generalization of local Lie group actions. This notion was first introduced by Lie at the end of the 19th century. Lie, Medolaghi and Vessiot then developed the foundations of the theory, [**42, 47, 68**], followed notably by Cartan, [**11**], and many others, [**24, 35, 36, 44, 60, 66**], during the 20th century. The present dissertation follows Olver and Pohjanpelto's more recent work, [**52**], and Thompson's Ph.D. thesis, [**67**].

The formal definitions of pseudo-groups and Lie pseudo-groups are given below for the sake of completeness. However, since they are somewhat technical, it is worth mentioning that, in this dissertation, all Lie pseudo-groups will be explicitly defined as local Lie group transformations potentially containing arbitrary functions.

Let $M$ be an $m$-dimensional manifold. A map $\varphi\colon M \to M$ is a local diffeomorphism[1] of $M$ if for any point $z \in \mathrm{dom}(\varphi)$ there is an open subset $U \subset \mathrm{dom}(\varphi)$ containing $z$ such that $\varphi\colon U \to \varphi(U)$ is a differentiable map with differentiable inverse. In the following, all transformations and underlying manifolds are assumed to be analytic so that Taylor series of diffeomorphisms converge.

**Definition 2.1.1.** A collection $\mathcal{G}$ of local diffeomorphisms of $M$ is a *pseudo-group* if

- $\mathcal{G}$ is closed under restriction: if $U \subset M$ is an open set and $g\colon U \to M$ is in $\mathcal{G}$, then so is the restriction $g|_V$ for all open $V \subset U$;
- elements of $\mathcal{G}$ can be pieced together: if $U_\nu \subset M$ are open subsets, $U = \bigcup_\nu U_\nu$, and $g\colon U \to M$ is a local diffeomorphism with $g|_{U_\nu} \in \mathcal{G}$ for all $\nu$, then $g \in \mathcal{G}$;
- $\mathcal{G}$ is closed under composition: if $g\colon U \to M$ and $h\colon V \to M$ are two diffeomorphisms belonging to $\mathcal{G}$, and $g(U) \subset V$, then $h \circ g \in \mathcal{G}$;
- $\mathcal{G}$ is closed under inversion: if $g\colon U \to M$ is in $\mathcal{G}$ then so is $g^{-1}\colon g(U) \to M$.

Bullets one and two reflect the topological properties of continuous groups while bullets three and four reflect the algebraic ones. Bullets three and four imply that $\mathcal{G}$ contains the identity diffeomorphism. These are analogues of the standard requirements for group actions. However, the composition of elements of $\mathcal{G}$ is not always defined since the composition $\psi \circ \varphi$ of two diffeomorphisms is defined only if $\mathrm{im}(\varphi) \subset \mathrm{dom}(\psi)$.

[1] This notation allows the domain of $\varphi$ to be an open subset of $M$

**Example 2.1.2.** One of the simplest pseudo-groups is given by the collection of all local diffeomorphisms $\mathcal{D} = \mathcal{D}(M)$ of a manifold $M$. All other pseudo-groups defined on $M$ are sub-pseudo-groups of $\mathcal{D}$.

**Example 2.1.3.** All global and local Lie group actions are pseudo-groups.

Global and local Lie group actions actually belong to a subclass of pseudo-groups called Lie pseudo-groups. In this thesis, we restrict our attention to Lie pseudo-groups. The formal definition of Lie pseudo-groups involves jets of local diffeormorphisms. In fact, jet spaces were invented for this purpose by Ehresmann, [**24**]. See [**48**] for a modern treatment. The following states the notational conventions used in this dissertation. Let $\varphi$ be a local diffeomorphism of $M$. The $n^{\text{th}}$ order jet $\varphi^{(n)}|_z$ of $\varphi$ at a point $z \in M$ is the equivalence class of diffeomorphisms sharing the same $n^{\text{th}}$ order Taylor polynomial at $z$. In the system of local coordinates $z = (z^1, \ldots, z^m) \in M$, let

$$\varphi(z) = (\varphi^1(z), \ldots, \varphi^m(z)).$$

The coordinates $z$ and $Z = \varphi(z)$ are called the source and target coordinates respectively of the diffeomorphism $\varphi$. Introducing the multi-index notation

$$J = (j^1, \ldots, j^m) \in \mathbb{N}^m,$$

the $n^{\text{th}}$ order polynomial expansion of $\varphi^a$ around $z_0$ is

$$P_n[\varphi^a, z](z_0) = \sum_{\#J=0}^{n} \frac{Z^a_J}{J!}(z - z_0)^J, \qquad a = 1, \ldots, m,$$

where

$$\#J = j^1 + \cdots + j^m, \qquad J! = j^1! \cdots j^m!, \qquad (z - z_0)^J = (z^1 - z_0^1)^{j^1} \cdots (z^m - z_0^m)^{j^m},$$

and

$$Z^a_J = \partial^J \varphi^a\big|_{z_0} = \left.\frac{\partial^{\#J}\varphi^a}{(\partial z^1)^{j^1} \cdots (\partial z^m)^{j^m}}\right|_{z_0}$$

denotes the derivatives of $\varphi^a$ evaluated at the point $z_0$. The equivalence class $\varphi^{(n)}|_z$ at the point $z$ is uniquely determined by the Taylor coefficients $Z^a_J$ and thus we write, by abuse of notation,

$$\varphi^{(n)}|_z = (z, Z^{(n)}),$$

where $Z^{(n)}$ denotes the collection of partial derivatives $Z^a_J$ of order $0 \leq \#J \leq n$. The set of all $\varphi^{(n)}|_z$ is noted $\mathcal{D}^{(n)}|_z = \{\varphi^{(n)}|_z\}$. The jet bundle

$$\mathcal{D}^{(n)} = \bigcup_{z \in M} \mathcal{D}^{(n)}|_z$$

denotes the set of $n^{\text{th}}$ order jets $\varphi^{(n)}|_z$ for all $z \in M$. The representatives $(z, Z^{(n)})$ of the $n^{\text{th}}$ order jets equivalence class are used as local coordinates in $\mathcal{D}^{(n)}$. For $k > n$ there is a natural projection $\widetilde{\pi}^k_n \colon \mathcal{D}^{(k)} \to \mathcal{D}^{(n)}$ corresponding to the truncation of Taylor polynomials

$$\varphi^{(k)}|_z = (z, Z^{(k)}) \overset{\widetilde{\pi}^k_n}{\mapsto} \varphi^{(n)}|_z = (z, Z^{(n)}).$$

**Example 2.1.4.** Let $M = \mathbb{R}$ and $\varphi$ be a local diffeomorphism of $\mathbb{R}$:

$$\begin{aligned} \varphi: \quad & \mathbb{R} \to \mathbb{R} \\ & x \mapsto X = \varphi(x). \end{aligned}$$

Local coordinates at $x$ for the second order jet can be given by $\varphi^{(2)}|_x = (x, X, X_x, X_{xx})$. For composition of diffeomorphisms, when defined, jets are computed using the chain rule. For example, if $\bar{X} = \psi(X)$, then

$$\begin{aligned} \bar{X}_x &= \psi(X)_x = \psi(X)_X X_x = \bar{X}_X X_x, \\ \bar{X}_{xx} &= (\bar{X}_x)_x = \bar{X}_X X_{xx} + \bar{X}_{XX} X_x^2, \end{aligned}$$

and thus local coordinates at $x$ for the second order jet of the composition $\psi \circ \varphi$ are given by

$$(\psi \circ \varphi)^{(2)}|_x = (x, \bar{X}, \bar{X}_X X_x, \bar{X}_X X_{xx} + \bar{X}_{XX} X_x^2).$$

Lie pseudo-groups are pseudo-groups whose elements are solutions of differential equations defined in the jet bundle $\mathcal{D}^{(n)}$. Let us start with some simple examples before tackling the formal definition.

**Example 2.1.5.** The set of translations

$$X = x + c, \qquad U = u, \tag{2.1.1}$$

with $c \in \mathbb{R}$, forms a Lie pseudo-group acting on $M = \mathbb{R}^2$. The group action (2.1.1) is closed under composition since if

$$X = x + c_1 \qquad \text{and} \qquad \bar{X} = X + c_2,$$

then

$$\bar{X} = x + (c_1 + c_2).$$

Inverses are obtained by taking $c_2 = -c_1$. Note that the group action (2.1.1) can be viewed as the solution of the system of differential equations

$$X_x = 1, \qquad X_u = 0, \qquad U = u, \tag{2.1.2}$$

defined in $\mathcal{D}^{(1)}$ with local coordinates $\varphi^{(1)}|_z = (x, u, X, U, X_x, X_u, U_x, U_u)$. Indeed, let $X = f(x, u)$ and $U = g(x, u)$ be a general point transformation of the plane. Equations (2.1.2) impose the following constraints on $f(x, u)$ and $g(x, u)$:

$$\begin{aligned} U = u \;&\Rightarrow\; U = g(x, u) = u, \\ X_u = 0 \;&\Rightarrow\; X = f(x, u) = f(x), \\ X_x = 1 \;&\Rightarrow\; X = f(x) = \int 1 dx = x + c. \end{aligned}$$

The set of translations of the preceding example forms a global Lie group action since it is defined for any $c \in \mathbb{R}$. However, some actions might only be defined locally as in the following example.

**Example 2.1.6.** The action on $M = \mathbb{R}^2$ given by

$$X = \frac{x}{1-\epsilon x}, \qquad U = \frac{u}{1-\epsilon x}, \tag{2.1.3}$$

with $|\epsilon| < \frac{1}{x}$, forms a Lie pseudo-group acting on $M = \mathbb{R}^2$. The pseudo-group action (2.1.3) is closed under composition since if

$$X = \frac{x}{1-\epsilon x} \qquad \text{and} \qquad \bar{X} = \frac{X}{1-\delta X},$$

then

$$\begin{aligned} \bar{X} &= \frac{\frac{x}{1-\epsilon x}}{1-\delta\frac{x}{1-\epsilon x}} \\ &= \frac{x}{1-\epsilon x-\delta x} \\ &= \frac{x}{1-(\epsilon+\delta)x} \end{aligned}$$

wherever defined, i.e. $|\epsilon+\delta| < \frac{1}{x}$. Inverses are obtained by taking $\delta = -\epsilon$. The pseudo-group (2.1.3) can be viewed as the solution of the system of differential equations

$$X_x = \frac{X^2}{x^2}, \qquad X_u = 0, \qquad U = X\frac{u}{x}, \tag{2.1.4}$$

which is again defined on $\mathcal{D}^{(1)}$. Indeed, the differential equations (2.1.4) impose the following constraints on $X = f(x,u)$ and $U = g(x,u)$:

$$\begin{aligned} X_u = 0 \;&\Rightarrow\; X = f(x,u) = f(x), \\ X_x = \frac{X^2}{x^2} \;\Rightarrow\; \frac{-1}{f(x)} = \frac{-1}{x} + \epsilon \;&\Rightarrow\; X = f(x) = \frac{x}{1-\epsilon x}, \\ U = X\frac{u}{x} \;&\Rightarrow\; U = \frac{u}{1-\epsilon x}. \end{aligned}$$

In the two previous examples, the pseudo-group actions contained a finite number of parameters (one in each case). These actions qualify as local Lie group actions. However, pseudo-group actions can also contain arbitrary functions as will show the next example. These actions, containing arbitrary functions, are not finite-dimensional Lie group actions and are the main reason the more general notion of pseudo-groups was introduced. In other words, the concept of pseudo-groups includes both finite and infinite-dimensional local Lie groups.

**Example 2.1.7.** The set of transformations of $\mathbb{R}^2$

$$X = f(x), \qquad U = \frac{u}{f'(x)}, \tag{2.1.5}$$

with $f \in \mathcal{D}(\mathbb{R})$, forms a Lie pseudo-group. It is worth noting that the algebra of this pseudo-group, which will be computed below, is none other than the Virasoro algebra without a central extension. The pseudo-group action (2.1.5) is closed under composition since if

$$X = f(x), \qquad U = \frac{u}{f'(x)}$$

and

$$\bar{X} = g(X), \qquad \bar{U} = \frac{U}{g'(X)},$$

then

$$\bar{X} = g(f(x)) = (g \circ f)(x), \qquad \bar{U} = \frac{u}{g'(f(x))f'(x)} = \frac{u}{(g \circ f)'(x)},$$

whenever $g \circ f$ is defined. Inverses are obtained by taking $g = f^{-1}$. Once again, the pseudo-group action (2.1.5) is the solution of a system of differential equations defined in $\mathcal{D}^{(1)}$, namely

$$X_u = 0, \qquad UX_x = u. \tag{2.1.6}$$

If, in general, $X = f(x,u)$ and $U = g(x,u)$, the constraints imposed by the equations (2.1.6) are as follows:

$$X_u = 0 \;\Rightarrow\; X = f(x,u) = f(x),$$
$$UX_x = u \;\Rightarrow\; U = \frac{u}{X_x} = \frac{u}{f'(x)}.$$

**Definition 2.1.8.** Let $\mathcal{G} \subset \mathcal{D}$ be a pseudo-group and $\mathcal{G}^{(n)}$ its collection of $n^{\text{th}}$ order jets. The pseudo-group $\mathcal{G}$ is called a *Lie pseudo-group* if there exists a $n^\star \geq 1$ such that for all $n \geq n^\star$:

- $\mathcal{G}^{(n)} \subset \mathcal{D}^{(n)}$ forms a smooth embedded subbundle;
- the projection $\widetilde{\pi}^{n+1}_n \colon \mathcal{G}^{(n+1)} \to \mathcal{G}^{(n)}$ is a fibration;
- every local diffeomorphism $g \in \mathcal{D}$ satisfying $g^{(n^\star)} \subset \mathcal{G}^{(n^\star)}$ belongs to $\mathcal{G}$;
- $\mathcal{G}^{(n)} = \mathrm{pr}^{(n-n^\star)}\mathcal{G}^{(n^\star)}$ is obtained by prolongation.

The lowest $n^\star$ for which the above properties hold is called the order of the Lie pseudo-group. Although Definition 2.1.8 might seem abstruse at first sight, everything becomes much simpler in local coordinates. In practice, all Lie pseudo-groups $\mathcal{G}$ are defined by identifying $\mathcal{G}^{(n)}$ to a system of differential equations on $\mathcal{D}^{(n)}$ as in the previous examples (see equations (2.1.2), (2.1.4) and (2.1.6)). The system of differential equations defining a Lie pseudo-group $\mathcal{G}$ is called the system of *determining equations* and is written

$$F^{(n)}(z, Z^{(n)}) = 0. \tag{2.1.7}$$

Each bullet of Definition 2.1.8 can be restated in terms of the *determining equations* (2.1.7). Bullet three states that any solution of the *determining equations* is an element of $\mathcal{G}$. Bullet four states that *determining equations* of order $n$ are obtained by prolonging (differentiating) the *determining equations* of order $n^\star$. The solution set of the *determing equations* is an embedded subbundle of $\mathcal{D}^{(n)}$ by construction (bullet one). Bullet two states that differentiating the *determining equations* to generate prolongations does not add any new information to the system. This requirement is related to the integrability of the *determining equations*.

**Example 2.1.9.** The *determining equations* of the translation pseudo-group treated in Example 2.1.5 are

$$F^{(1)}(x,u,X,U,X_x,X_u,U_x,U_u) = \begin{cases} X_x = 1, \qquad X_u = 0, \\ U = u, \qquad U_x = 0, \qquad U_u = 1. \end{cases} \tag{2.1.8}$$

The equations $U_x = 0$ and $U_u = 1$ are simply the derivatives of $U = u$. Since they add no new information, they are not absolutely necessary to characterize the pseudo-group and are often omitted in practice as in Example 2.1.5 (Equation (2.1.2)). As prescribed by Bullet four of Definition 2.1.8, it suffices to differentiate the determining equations of order 1 to obtain the system of determining equations of order $n = 2$:

$$F^{(2)}(z,Z^{(2)}) = \begin{cases} X_x = 1, \quad X_u = 0, \quad U = u, \quad U_x = 0, \quad U_u = 1, \\ X_{xx} = 0, \quad X_{xu} = 0, \quad X_{uu} = 0, \\ U_{xx} = 0, \quad U_{xu} = 0, \quad U_{uu} = 0, \end{cases} \tag{2.1.9}$$

where $z = (x,u)$ and $Z^{(2)} = (X,U,X_x,X_u,U_x,U_u,X_{xx},X_{xu},X_{uu},U_{xx},U_{xu},U_{uu})$. The *determining equations* of order two and all subsequent orders do not add any new constraints on the local diffeomorphisms $X = X(x,u)$ and $U = U(x,u)$ (being the derivatives of the *determining equations* of order 1). This information is encoded in the second bullet of Definition 2.1.8. The order of the pseudo-group (2.1.1) is thus $n^\star = 1$ since the equations $X_x = 1$ and $X_u = 0$ are needed and belong to the first order jet. Equations (2.1.8) and their prolongation form a system of equations on $\mathcal{D}^{(n)}$ and their solutions are thus a smooth embedded submanifold of $\mathcal{D}^{(n)}$ by construction (this satisfies bullet one). All solutions of the system (2.1.8) and its prolongations are generated by the prolongation of the action

$$X = x + c, \qquad U = u, \tag{2.1.10}$$

and so the action (2.1.10) respects bullets three and four.

**Example 2.1.10.** The *determining equations* of the pseudo-group treated in Example 2.1.6 are

$$F^{(1)}(z, Z^{(1)}) = \begin{cases} X_x = \frac{X^2}{x^2}, \qquad X_u = 0, \\ U = X\frac{u}{x}, \qquad U_x = (X-x)\frac{uX}{x^3}, \qquad U_u = \frac{X}{x}, \end{cases} \tag{2.1.11}$$

where the equations for $U_x$ and $U_u$ are obtained by differentiating $U$ and using the fact that $X_x = \frac{X^2}{x^2}$. The system of *determining equations* of order $n = 2$ is given by differentiating the determining equations of order 1 and the result is:

$$F^{(2)}(z, Z^{(2)}) = \begin{cases} X_x = 1, \quad X_u = 0, \quad U = X\frac{u}{x}, \qquad U_x = (X-x)\frac{uX}{x^3}, \qquad U_u = \frac{X}{x}, \\ X_{xx} = 2(X-x)\frac{X^2}{x^4}, \quad X_{xu} = 0, \quad X_{uu} = 0, \\ U_{xx} = 2(X^2 - 2xX + x^2)\frac{uX}{x^5}, \quad U_{xu} = 0, \quad U_{uu} = 0. \end{cases} \tag{2.1.12}$$

Once again, the *determining equations* of order 2 add no new constraints on the solutions $X$ and $U$ (bullet two) and all the solutions of the *determining equations* of order $n$ are given by prolonging the solutions of the *determining equations* of order 1 (2.1.11) given by the action (2.1.3) (bullets three and four).

A Lie pseudo-group is said to be of *finite type* if the solution space of (2.1.7) only involves a finite number of arbitrary constants (as in Example 2.1.5 and Example 2.1.6). Lie pseudo-groups of finite type are local Lie group actions. On the other hand, a Lie pseudo-group is of *infinite type* if it involves arbitrary functions (as in Example 2.1.7).

While in this dissertation Lie pseudo-groups are characterized by their *determining equations* and their corresponding pseudo-group actions, another common way to characterize them is to use Lie algebras. The following explains how to transition from the pseudo-group action to its Lie algebra generators.

The Taylor expansion of a diffeomorphism around the identity transformation is

$$Z^a = z^a + \epsilon\zeta^a(z) + O(\epsilon^2), \tag{2.1.13}$$

where $\epsilon$ is some small parameter. Substituting the Taylor series (2.1.13) into the *determining equations* (2.1.7), differentiating with respect to $\epsilon$ and then setting $\epsilon = 0$ yields the *infinitesimal determining equations*

$$L^{(n)}(z, \zeta^{(n)}) = 0. \tag{2.1.14}$$

A local vector field

$$\mathbf{v} = \sum_{a=1}^{m} \zeta^a(z)\frac{\partial}{\partial z^a} \tag{2.1.15}$$

is in the Lie algebra $\mathfrak{g}$ of infinitesimal generators of $\mathcal{G}$ if its components $\zeta^a(z)$ are solutions of the *infinitesimal determining equations* (2.1.14).

**Remark 2.1.11.** Given a differential equation $\Delta(x, u^{(n)}) = 0$ with symmetry pseudo-group $\mathcal{G}$, the *infinitesimal determining equations* (2.1.14) are equivalent to the equations obtained by Lie's standard algorithm for determining the symmetry algebra of the differential equation $\Delta(x, u^{(n)}) = 0$, [**48**].

In the following examples, since only terms of order $\epsilon$ end up affecting the Lie algebras and their *infinitesimal determining equations*, we omit terms of order $O(\epsilon^2)$ and write

$$Z^a = z^a + \epsilon\zeta^a(z)$$

by abuse of notation.

**Example 2.1.12.** The *determining equations* of the translations treated in Example 2.1.5 are

$$F^{(1)}(x,u,X,U,X_x,X_u,U_x,U_u) = \begin{cases} X_x = 1, \qquad X_u = 0, \\ U = u, \qquad U_x = 0, \qquad U_u = 1. \end{cases} \tag{2.1.16}$$

The *infinitesimal determining equations* are obtained by substituting $X = x + \epsilon\xi$ and $U = u + \epsilon\varphi$ in the *determining equations* (2.1.16), differentiating with respect to $\epsilon$ and setting $\epsilon = 0$. Explicitly, the substitution yields

$$\begin{aligned} X_x = (x+\epsilon\xi)_x = 1 + \epsilon\xi_x = 1 &\Rightarrow \epsilon\xi_x = 0, \\ X_u = (x+\epsilon\xi)_u = \epsilon\xi_u = 0 &\Rightarrow \epsilon\xi_u = 0, \\ U = u + \epsilon\varphi = u &\Rightarrow \epsilon\varphi = 0, \\ U_x = \epsilon\varphi_x = 0 &\Rightarrow \epsilon\varphi_x = 0, \\ U_u = \epsilon\varphi_u = 1 &\Rightarrow \epsilon\varphi_u = 1, \end{aligned}$$

and, differentiating with respect to $\epsilon$, the *infinitesimal determining equations* are

$$L^{(1)}(x,u,\xi,\varphi,\xi_x,\xi_u,\varphi_x,\varphi_u) = \begin{cases} \xi_x = \xi_u = 0 \\ \varphi = \varphi_x = \varphi_u = 0. \end{cases} \tag{2.1.17}$$

A local vector field

$$\mathbf{v} = \xi(x,u)\frac{\partial}{\partial x} + \varphi(x,u)\frac{\partial}{\partial u}$$

is an infinitesimal generator of the local group action if $\xi$ and $\varphi$ form a solution of the *infinitesimal determining equations* (2.1.17), namely

$$\mathbf{v} = \partial_x$$

up to a multiplicative constant.

**Example 2.1.13.** As a slightly more challenging exercice, let us find the *infinitesimal determining equations* for Example 2.1.6 using the same procedure as above. The *determining equations* are

$$F^{(1)}(x,u,X,U,X_x,X_u,U_x,U_u) = \begin{cases} X_x = \frac{X^2}{x^2}, & X_u = 0, \\ U = X\frac{u}{x}, & U_x = (X-x)\frac{uX}{x^3}, \qquad U_u = \frac{X}{x}. \end{cases} \tag{2.1.18}$$

Substituting $X = x + \epsilon\xi$ and $U = u + \epsilon\varphi$ in the *determining equations* (2.1.18) yields

$$X_x = 1 + \epsilon\xi_x = 1 + \epsilon\frac{2\xi}{x},$$

$$X_u = \epsilon\xi_u = 0,$$

$$U = u + \epsilon\varphi = (x + \epsilon\xi)\frac{u}{x}.$$

The equations for $U_x$ and $U_u$ can be omitted since they were derived from the equation for $U$. Differentiating with respect to $\epsilon$ and setting $\epsilon = 0$ gives the *infinitesimal determining equations*:

$$L^{(1)}(x,u,\xi,\varphi,\xi_x,\xi_u,\varphi_x,\varphi_u) = \begin{cases} \xi_x = 2\frac{\xi}{x}, & \xi_u = 0 \\ \varphi = \xi\frac{u}{x}, & \varphi_x = (\xi_x - \xi)\frac{u}{x^2}, \qquad \varphi_u = \frac{\xi}{x}, \end{cases} \tag{2.1.19}$$

where the equations for $\varphi_x$ and $\varphi_u$ can be obtained by differentiating the equation for $\varphi$. Integrating the system of *infinitesimal determining equations* (2.1.19) to find $\xi$ and $\varphi$ gives the infinitesimal generator of this local Lie group action:

$$\mathbf{v} = x^2\partial_x + xu\partial_u \tag{2.1.20}$$

up to a multiplicative constant.

**Example 2.1.14.** As a final example let us calculate the *infinitesimal determining equations* and infinitesimal generators for the Lie pseudo-group of Example 2.1.7.

The *determining equations are*

$$F^{(1)}(x,u,X,U,X_x,X_u,U_x,U_u)=\begin{cases}X_u=0,\\ UX_x=u, \qquad U_u\,X_x=1.\end{cases} \tag{2.1.21}$$

Substituting $X=x+\epsilon\xi$ and $U=u+\epsilon\varphi$ in the *determining equations* yields

$$\begin{aligned}(x+\epsilon\xi)_u&=\epsilon\xi_u=0,\\ (u+\epsilon\varphi)(x+\epsilon\xi)_x&=(u+\epsilon\varphi)(1+\epsilon\xi_x)=u\Rightarrow\epsilon(\varphi+u\xi_x)=0,\\ (u+\epsilon\varphi)_u(x+\epsilon\xi)_x&=(1+\epsilon\varphi_u)(1+\epsilon\xi_x)=1\Rightarrow\epsilon(\varphi_u+\xi_x)=0.\end{aligned} \tag{2.1.22}$$

Differentiating the equations (2.1.22) with respect to $\epsilon$ and then setting $\epsilon=0$ gives the *infinitesimal determining equations*

$$L^{(1)}(x,u,\xi,\varphi,\xi_x,\xi_u,\varphi_x,\varphi_u)=\begin{cases}\xi_u=0,\\ \varphi=-u\xi_x, \qquad \varphi_u=-\xi_x,\end{cases} \tag{2.1.23}$$

and the general solution is

$$\mathbf{v}=a(x)\frac{\partial}{\partial x}-u\,a'(x)\frac{\partial}{\partial u},$$

where $a(x)$ is any smooth function ($a(x)$ should be analytic if one needs Taylor series to converge).

## 2.2. Pseudo-group action and the search for invariants

Let $z=(x,u)$ be coordinates on $M$ and $\mathrm{J}^{(n)}$ be the space with coordinates

$$z^{(n)}=(x,u^{(n)}), \tag{2.2.1}$$

where $x$ denotes the collection of the independent variables and $u^{(n)}$ denotes the collection of the dependent variables and all their derivatives up to order $n$ with respect to the independent variables $x$. Let $p$ be the number of independent variables and $q$ the number of dependent variables. The capital $J$ still also denotes the multi-index[2]

$$J = (j^1, j^2, \ldots, j^p) \in \mathbb{N}^p$$

with

$$\#J = j^1 + j^2 + \ldots + j^p.$$

Using this notation, all the partial derivatives of the dependent variables with respect to the independent variables are written

$$u^\alpha_{x^J} = D^J_x u^\alpha = D^{j^1}_{x^1} \ldots D^{j^p}_{x^p} u^\alpha = \frac{\partial^{\#J} u^\alpha}{(\partial x^1)^{j^1} \cdots (\partial x^p)^{j^p}}, \qquad 1 \leq \alpha \leq q. \tag{2.2.2}$$

The collection $u^{(n)}$ is thus the set of all the expressions $u^\alpha_{x^J}$ such that $0 \leq \#J \leq n$. The space $\mathrm{J}^{(n)}$ is called the $n^{\text{th}}$ order *submanifold jet bundle.*

**Example 2.2.1.** Consider the heat equation in one spatial dimension

$$u_t = u_{xx}.$$

The graphs of the solutions $u = u(x,t)$ live in a 3-dimensional space with coordinates $(x, t, u)$ and the second order submanifold jet bundle $\mathrm{J}^{(2)}$ coordinates are given by

$$(x, t, u, u_x, u_t, u_{xx}, u_{xt}, u_{tt}).$$

Differential invariants of order up to $n$ for a given pseudo-group are functions $I : \mathrm{J}^{(n)} \to \mathbb{R}$ which are preserved by the pseudo-group action. To define "preserve" formally, it is necessary to define clearly how pseudo-groups act on $\mathrm{J}^{(n)}$. The following explains how to act on $\mathrm{J}^{(n)}$ with $\mathcal{G}^{(n)}$ and how it enables one to find the differential invariants.

[2]The multi-index capital $J$ should not be mistaken with $\mathrm{J}^{(n)}$. This notation is unfortunate but it is standard in the litterature.

Given a pseudo-group $\mathcal{G}$ acting on a manifold $M$, there is an induced action of $\mathcal{G}^{(n)}$ on $\mathrm{J}^{(n)}$ given by the usual prolonged action:

$$g^{(n)} \cdot (x, u^{(n)}) = (X, U^{(n)}), \qquad \text{where defined,}$$

and where $X$ and $U$ are given by the pseudo-group action while $U^{(n)}$ is the collection of derivatives of the target dependent variables $U$ with respect to the target independent variables $X$ up to order $n$. The target derivatives $U^{(n)}$ are easily computed using the chain rule as demonstrated below. Using the same notation as for the source coordinates, the derivatives of the target coordinates are written

$$U^{\alpha}_{X^J} = D^J_X U^{\alpha} = D^{j^1}_{X^1} \ldots D^{j^p}_{X^p} U^{\alpha}, \qquad \alpha = 1, \ldots, q, \quad 0 \le \#J \le n,$$

and the target total derivative operators $D_{X^k}$, $1 \le k \le p$, are obtained as follows. The chain rule implies

$$U_{x^i} = \sum_{k=1}^{p} (D_{x^i} X^k) U_{X^k}, \qquad i = 1, \ldots, p,$$

or, in terms of the total derivative operators,

$$D_{x^i} = \sum_{k=1}^{p} (D_{x^i} X^k) D_{X^k}, \qquad i = 1, \ldots, p. \tag{2.2.3}$$

The system of linear equations (2.2.3) can be written, in matrix formulation,

$$\begin{pmatrix} D_{x^1} \\ \vdots \\ D_{x^p} \end{pmatrix} = B \begin{pmatrix} D_{X^1} \\ \vdots \\ D_{X^p} \end{pmatrix},$$

where $B$ is the jacobian matrix with entries $B_i^k = D_{x^i} X^k$. The target total derivatives $D_{X^k}$ are then given by inverting the jacobian matrix:

$$\begin{pmatrix} D_{X^1} \\ \vdots \\ D_{X^p} \end{pmatrix} = B^{-1} \begin{pmatrix} D_{x^1} \\ \vdots \\ D_{x^p} \end{pmatrix}.$$

Once the target total derivatives $D_{X^k}$ are known, the prolonged action of $\mathcal{G}^{(n)}$ on $\mathrm{J}^{(n)}$ is obtained by successive applications of the derivatives $D_{X^k}$ to $U$.

**Example 2.2.2.** Let a pseudo-group $\mathcal{G}$ act on surfaces in $\mathbb{R}^3$ expressed in local coordinates $(x, y, u(x, y))$. Using the chain rule, the first order derivatives of $U$ with respect to the independent source coordinates are given by

$$U_x = X_x\, U_X + Y_x\, U_Y, \qquad U_y = X_y\, U_X + Y_y\, U_Y.$$

Recasted in matrix formulation for the total derivative operators, the system is

$$\begin{pmatrix} D_x \\ D_y \end{pmatrix} = B \begin{pmatrix} D_X \\ D_Y \end{pmatrix}, \qquad \text{where} \qquad B = \begin{pmatrix} X_x & Y_x \\ X_y & Y_y \end{pmatrix}.$$

This implies

$$\begin{pmatrix} D_X \\ D_Y \end{pmatrix} = B^{-1} \begin{pmatrix} D_x \\ D_y \end{pmatrix}, \qquad \text{where} \qquad B^{-1} = \frac{1}{X_x\, Y_y - X_y\, Y_x} \begin{pmatrix} Y_y & -Y_x \\ -X_y & X_x \end{pmatrix}.$$

The target derivatives $U_X$ and $U_Y$ are thus

$$U_X = \frac{Y_y\, U_x - Y_x\, U_y}{X_x\, Y_y - X_y\, Y_x}, \qquad U_Y = \frac{X_x\, U_y - X_y\, U_x}{X_x\, Y_y - X_y\, Y_x}.$$

In particular, for the pseudo-group

$$X = f(x), \qquad Y = g(y), \qquad U = \frac{u}{f_x\, g_y}, \tag{2.2.4}$$

discussed in Chapter 4 (equation (**??**)), the jacobian matrix is given by

$$B = \begin{pmatrix} X_x & Y_x \\ X_y & Y_y \end{pmatrix} = \begin{pmatrix} f_x & 0 \\ 0 & g_y \end{pmatrix}$$

and its inverse by

$$B^{-1} = \frac{1}{f_x\, g_y} \begin{pmatrix} g_y & 0 \\ 0 & f_x \end{pmatrix}.$$

The target total derivative operators are thus

$$D_X = \frac{D_x}{f_x}, \qquad D_Y = \frac{D_y}{g_y}.$$

Acting with these operators on $U = \dfrac{u}{f_x\, g_y}$ yields the prolongation of the action on first order derivatives:

$$\begin{aligned} U_X &= \frac{1}{f_x} \cdot \frac{f_x\, g_y\, u_x - u\, f_{xx}\, g_y}{f_x^2\, g_y^2} = \frac{u_x\, f_x - u\, f_{xx}}{f_x^3\, g_y} \\ U_Y &= \frac{1}{g_y} \cdot \frac{f_x\, g_y\, u_y - u\, g_{yy}\, f_x}{f_x^2\, g_y^2} = \frac{u_y\, g_y - u\, g_{yy}}{f_x\, g_y^3}. \end{aligned}$$

It is now possible to give a formal definition of differential invariants.

**Definition 2.2.3.** A *differential invariant* is a differential function $I \colon \mathrm{J}^{(n)} \to \mathbb{R}$ which is unaffected by the prolonged action of $\mathcal{G}^{(n)}$ on $\mathrm{J}^{(n)}$, and so

$$I(X, U^{(n)}) = I(g^{(n)} \cdot (x, u^{(n)})) = I(x, u^{(n)}) \qquad \forall (x, u^{(n)}) \in \mathrm{J}^{(n)},\ \forall g^{(n)} \in \mathcal{G}^{(n)},$$

where defined.

**Example 2.2.4.** The differential function

$$I(x, u^{(n)}) = \frac{u\, u_{xy} - u_x\, u_y}{u^3}$$

is a differential invariant of the pseudo-group (2.2.4). To see this, let us compute the action on $u_{xy}$ using what we learned from the previous example:

$$\begin{aligned} U_{XY} = D_Y(U_X) &= \frac{D_y}{g_y}\left(\frac{u_x\, f_x - u\, f_{xx}}{f_x^3\, g_y}\right) \\ &= \frac{u_{xy}\, f_x\, g_y - u_y\, f_{xx}\, g_y - u_x\, f_x\, g_{yy} + u\, f_{xx}\, g_{yy}}{f_x^3\, g_y^3}. \end{aligned}$$

Thus, using again the expressions from last example,

$$\begin{aligned} I(X, U^{(n)}) &= \frac{U\, U_{XY} - U_X\, U_Y}{U^3} \\ &= \big(u\, u_{xy}\, f_x\, g_y - u\, u_y\, f_{xx}\, g_y - u\, u_x\, f_x\, g_{yy} + u^2\, f_{xx}\, g_{yy} \\ &\quad - u_x\, u_y\, f_x\, g_y + u\, u_y\, f_{xx}\, g_y + u\, u_x\, f_x\, g_{yy} - u^2\, f_{xx}\, g_{yy}\big) / \big(u^3\, f_x\, g_y\big) \\ &= \frac{u\, u_{xy} - u_x\, u_y}{u^3} \\ &= I(x, u^{(n)}), \end{aligned}$$

and $I$ is a differential invariant of the pseudo-group (2.2.4).

**Definition 2.2.5.** A system of equations $\Delta(x, u^{(n)}) = 0$ is invariant under a pseudo-group action $\mathcal{G}$ if its solution space is unaffected by the prolonged action of $\mathcal{G}^{(n)}$ on $\mathrm{J}^{(n)}$, and so

$$\Delta(g^{(n)} \cdot (x, u^{(n)})) = 0 \qquad \text{whenever } \Delta(x, u^{(n)}) = 0, \qquad \forall g^{(n)} \in \mathcal{G}^{(n)}$$

such that the action is defined.

**Example 2.2.6.** The differential equation

$$\frac{u\, u_{xy} - u_x\, u_y}{u^3} = 1$$

involving the differential function from Example 2.2.4 is invariant under the pseudo-group action (2.2.4) since it is built using solely invariants of the action. This equation will be further studied along this dissertation. It is the Liouville equation up to a change of variables given by $u = e^v$.

As the next example shows, invariant equations can arise without being built up from differential invariants of an action.

**Example 2.2.7.** Consider the differential equation

$$u_{xx} = 0. \tag{2.2.5}$$

The differential function $u_{xx}$ is clearly not an invariant of the dilations

$$X = x, \qquad U = \lambda u.$$

However, the differential equation (2.2.5) is invariant since

$$U_{XX}|_{u_{xx}=0} = \lambda u_{xx}|_{u_{xx}=0} = 0.$$

Before establishing an algorithm to find differential invariants of pseudo-groups, the following introduces a change of variables between the standard variables $(x, u)$ and so-called *computational variables*, [**28**], which will be represented by the letter $s$. These variables are usually chosen to be orthogonal in order to offer a cartesian frame of reference while the standard variables are free to be curvilinear. In the same spirit, computational variables were introduced in numerical analysis to build orthogonal and uniform meshes in situations were the original meshes were skewed. They will be used for a similar purpose here since pseudo-groups will act on meshes, deforming them, and it will be useful to have an orthonormal frame of reference unaffected by these transformations.

A submanifold $S \subset M$ can be parametrized by $p$ variables $s = (s^1, \ldots, s^p) \in \mathbb{R}^p$ so that

$$z(s) = (x(s), u(s)) \in S. \tag{2.2.6}$$

Let $\mathcal{J}^{(n)}$ be the space with local coordinates

$$\mathfrak{z}^{(n)} = (s, x^{(n)}, u^{(n)}) = (\ \ldots\ s^i\ \ldots\ x^i_{s^J}\ \ldots\ u^\alpha_{s^J}\ \ldots), \tag{2.2.7}$$

with $1 \leq i \leq p$, $1 \leq \alpha \leq q$, $0 \leq \#J \leq n$, and where the partial derivatives are defined as in (2.2.2) but with the standard variables $x$ replaced by the *computational variables* $s$. The space $\mathcal{J}^{(n)}$ is called the $n^{\text{th}}$ order *submanifold jet bundle in computational variables.* In $\mathcal{J}^{(n)}$, the computational variables $s^i$ play the role of the independent variables and $x^{(n)}$ and $u^{(n)}$ are the collections of partial derivatives up to order $n$ of the standard variables $x^i$and $u^\alpha$ with respect to the computational variables $s^i$. From now on, the variables appearing in $\mathrm{J}^{(n)}$ and $\mathcal{J}^{(n)}$ will be referred to as standard and computational variables respectively. The partial derivatives with respect to the new independent variables $s$ are given by the chain rule since the dependence of $u$ on $s$ follows from the original dependence of $u$ on $x$ $(u = u(x(s)))$. Explicitly, the total derivative operators are given by

$$D_{s^i} = \sum_{k=1}^{p} (D_{s^i} x^k) D_{x^k}, \qquad 1 \leq i \leq p,$$

which can be inverted if

$$\det(D_{s^i} x^k) \neq 0. \tag{2.2.8}$$

**Example 2.2.8.** Consider the case of two independent variables $(x, y)$ and one dependent variable $u(x, y)$. Introducing the computational variables $(s, t)$ so that $x(s, t)$, $y(s, t)$ and $u(x(s, t), y(s, t))$. We have that

$$u_s = x_s\, u_x + y_s\, u_y, \qquad u_t = x_t\, u_x + y_t\, u_y.$$

The corresponding total derivative operators are

$$D_s = x_s\, D_x + y_s\, D_y, \qquad D_t = x_t\, D_x + y_t\, D_y. \tag{2.2.9}$$

If

$$\begin{vmatrix} x_s & y_s \\ x_t & y_t \end{vmatrix} \neq 0,$$

the system (2.2.9) is invertible and

$$D_x = \frac{y_t\, D_s - y_s\, D_t}{x_s\, y_t - x_t\, y_s}, \qquad D_y = \frac{x_s\, D_t - x_t\, D_s}{x_s\, y_t - x_t\, y_s}. \tag{2.2.10}$$

Given a Lie pseudo-group $\mathcal{G}$ acting on $M$, the action is prolonged to the computational variables by requiring that they remain unchanged:

$$g \cdot (s, z) = (s, g \cdot z) \qquad \text{for all} \qquad g \in \mathcal{G}.$$

By abuse of notation, we still use $\mathcal{G}$ to denote the extended action $\{\mathbb{1}\} \times \mathcal{G}$ on $\mathbb{R}^p \times M$.

The induced action of the pseudo-group $\mathcal{G}^{(n)}$ is now

$$g^{(n)} \cdot \mathfrak{z}^{(n)} = g^{(n)} \cdot (s, x^{(n)}, u^{(n)}) = (s, X^{(n)}, U^{(n)}) = \mathfrak{Z}^{(n)}, \qquad \text{where defined},$$

and where $X^{(n)}$ and $U^{(n)}$ are the collections of derivatives of the target variables with respect to the computational variables up to order $n$, namely

$$\begin{aligned} X^\alpha_{s^J} &= D^J_s X^\alpha = D^{j^1}_{s^1} \ldots D^{j^p}_{s^p} X^\alpha, \qquad \alpha = 1, \ldots, p, \\ U^\beta_{s^J} &= D^J_s U^\beta = D^{j^1}_{s^1} \ldots D^{j^p}_{s^p} U^\beta, \qquad \beta = 1, \ldots, q, \quad 0 \leq \#J \leq n. \end{aligned}$$

**Example 2.2.9.** Consider the pseudo-group $\mathcal{G}$

$$X = f(x), \qquad Y = y, \qquad U = \frac{u}{f'(x)}, \tag{2.2.11}$$

acting on surfaces in $\mathbb{R}^3$ expressed in local coordinates $(x, y, u(x, y))$. Introducing computational variables $(s, t)$, the derivatives of the target coordinates $(X, Y, U)$ with respect to computational variables $(s,t)$ are computed by differentiating Equations (2.2.11) using the chain rule and considering $(x,y,u)$ to be functions of $s$ and $t$. To simplify calculations, let the relations between standard and computational variables be constrained by

$$x = x(s), \qquad y = kt + y_0, \tag{2.2.12}$$

where $k > 0$ and $y_0$ are constants (the same constraints will be used in Example 2.2.15). The first order derivatives of the target coordinates with respect to computational variables are thus

$$X_s = f_x\, x_s, \qquad Y_t = k, \qquad U_s = \frac{u_s}{f_x} - \frac{u\, f_{xx}\, x_s}{f_x^2}, \qquad U_t = \frac{u_t}{f_x},$$

from which it is possible to write down the induced action of $\mathcal{G}^{(1)}$ on $\mathcal{J}^{(1)}$:

$$\begin{gathered} S = s, \qquad T = t, \qquad Y = y, \qquad X = f(x), \qquad U = \frac{u}{f_x}, \\ X_s = f_x\, x_s, \qquad Y_t = k, \qquad U_s = \frac{u_s}{f_x} - \frac{u\, f_{xx}\, x_s}{f_x^2}, \qquad U_t = \frac{u_t}{f_x}. \end{gathered} \tag{2.2.13}$$

The notion of differential invariants and invariant equations are readily generalized to computational variables. Both definitions remain the same except for the fact that the standard variables jet bundle $\mathrm{J}^{(n)}$ is replaced by the computational variables jet bundle $\mathcal{J}^{(n)}$. Explicitly, differential invariants in computational variables are differential functions $I\colon \mathcal{J}^{(n)} \to \mathbb{R}$ unaffected by the pseudo-group action, i.e. $I(s, X^{(n)}, U^{(n)}) = I(s, x^{(n)}, u^{(n)})$, while invariant equations are equations such that

$$\Delta(g^{(n)} \cdot (s, x^{(n)}, u^{(n)})) = 0 \qquad \text{whenever} \quad \Delta(s, x^{(n)}, u^{(n)}) = 0, \quad \forall g^{(n)} \in \mathcal{G}^{(n)},$$

whenever the action is defined.

**Remark 2.2.10.** The relations (2.2.12) were not chosen completely arbitrarily. They are solutions of a system of differential equations invariant under the pseudo-group action, namely

$$x_t = 0, \qquad y_s = 0, \qquad y_t = k.$$

The equations $y_s = 0$ and $y_t = k$ are invariants since $y$, $t$, and $s$ are invariants of the action. The invariance of $x_t = 0$ follows from the chain rule:

$$X_t = f_x \, x_t = 0 \qquad \text{when} \qquad x_t = 0.$$

The non-degeneracy condition (2.2.8) requires the invariant constraint $x_s \neq 0$ to be satisfied.

I will now recast how to construct a moving frame, [**54**], in the framework of computational variables. Moving frames were first developed by Cartan, [**9, 10**], and they are a powerful tool with many applications in differential geometry. In this thesis, they will be the means to construct differential invariants.

**Definition 2.2.11.** Let $\mathcal{G}$ be a pseudo-group acting on a manifold $M$. A *(right) moving frame* is a smooth map $\rho : M \to \mathcal{G}$ such that

$$\rho(g \cdot z) = \rho(z) \cdot g^{-1}, \qquad \forall g \in \mathcal{G}|_z.$$

If the action of $\mathcal{G}^{(n)}$ on $\mathcal{J}^{(n)}$ is considered, a map

$$\rho^{(n)}(g^{(n)} \cdot \mathfrak{z}^{(n)}) = \rho^{(n)}(\mathfrak{z}^{(n)}) \cdot g^{(n)-1}, \qquad \forall g^{(n)} \in \mathcal{G}^{(n)}|_{\mathfrak{z}},$$

is called a *(right) moving frame* of order $n$.

If $\rho^{(n)}$ is a *(right) moving frame of order* $n$, each component of $\rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)}$ is an invariant since:

$$\begin{aligned} g^{(n)} \cdot \big(\rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)}\big) &= \rho^{(n)}(g^{(n)} \cdot \mathfrak{z}^{(n)}) \cdot (g^{(n)} \cdot \mathfrak{z}^{(n)}) \\ &= \rho^{(n)}(\mathfrak{z}^{(n)}) \cdot g^{(n)^{-1}} \cdot g^{(n)} \cdot \mathfrak{z}^{(n)} \qquad \text{by definition of } \rho^{(n)} \\ &= \rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)}. \end{aligned}$$

**Proposition 2.2.12.** The application of the moving frame map to all local coordinates

$$\rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)}$$

forms a complete set of differential invariants of order $\leq n$. This *invariantization* of the local coordinates is also written

$$\iota(s, x^{(n)}, u^{(n)}) \equiv \rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)}.$$

The invariantization of an arbitrary function $F$ of local coordinates is given by the function evaluated at the invariantized coordinates $\iota F(\mathfrak{z}^{(n)}) = F(\iota(\mathfrak{z}^{(n)}))$.

Geometrically, in the jet bundle $\mathcal{J}^{(n)}$, a moving frame is defined by choosing a submanifold $\mathcal{K}^{(n)}$, called a *cross-section*, intersecting all the pseudo-group orbits transversally. At $\mathfrak{z}^{(n)}$, $\rho^{(n)}(\mathfrak{z}^{(n)})$ is the transformation sending $\mathfrak{z}^{(n)}$ onto the *cross-section*, i.e. $\rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)} \in \mathcal{K}^{(n)}$ (see Figure 2.1).

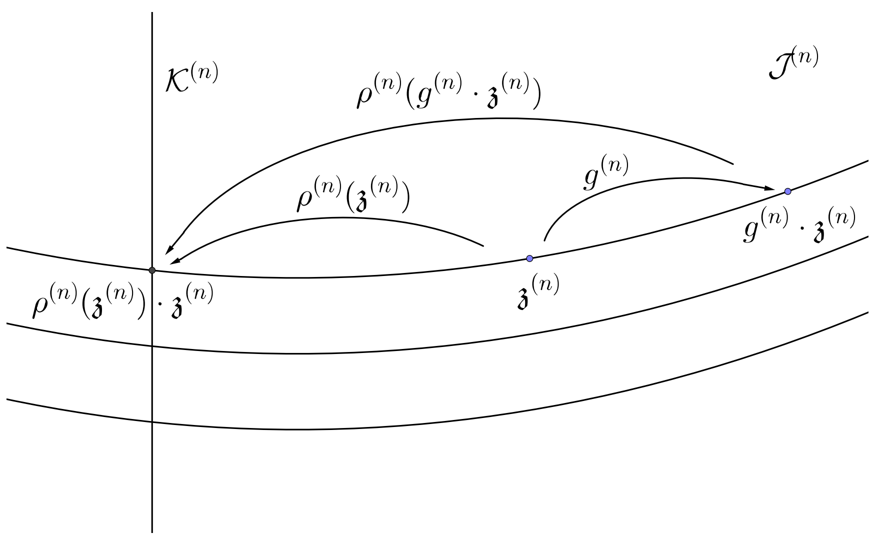


FIG. 2.1. The $\mathcal{G}$-equivariant map $\rho^{(n)}$ in $\mathcal{J}^{(n)}$.

Choosing a *cross-section*

$$\mathcal{K}^{(n)} = \{\mathfrak{z}_{i_1} = c_1, \ldots, \mathfrak{z}_{i_l} = c_l\}, \qquad l = \dim(\mathcal{G}^{(n)}|_{\mathfrak{z}}), \tag{2.2.14}$$

where the $\mathfrak{z}_{i_m}$ stand for some local coordinates in $\mathcal{J}^{(n)}$ (such as $x$, $u$, $u_x$ and so on), and solving the *normalization equations*

$$\rho^{(n)}(\mathfrak{z}_{\mathrm{i}_1}) = \mathfrak{Z}_{i_1}(s, x^{(n)}, u^{(n)}, g^{(n)}) = c_1, \quad \ldots, \quad \rho^{(n)}(\mathfrak{z}_{\mathrm{i}_l}) = \mathfrak{Z}_{i_l}(s, x^{(n)}, u^{(n)}, g^{(n)}) = c_l,$$

for the pseudo-group parameters $g^{(n)}$ defines the moving frame map $\rho^{(n)}$. The *cross-section* $\mathcal{K}^{(n)}$ must be chosen so that there is enough independent equations in the *normalization equations* to solve for all the pseudo-group parameters $g^{(n)}$ (this is why $l = \dim(\mathcal{G}^{(n)}|_{\mathfrak{z}})$). Our capacity to find differential invariants is thus conditioned by the solvability of a system of algebraic equations (the *normalization equations*) for the pseudo-group parameters.

Another common way to find differential invariants is to search for differential functions annihilated by infinitesimal generators of Lie algebras, [**48**]. This involves the resolution of partial differential equations. While both methods (using the group or its algebra) are equivalent, one of them is often easier to apply depending on the situation. In this thesis, the moving frame approach is always used although it is possible to do all the computations using Lie algebras.

**Example 2.2.13.** Let us look back at the pseudo-group

$$X = \frac{x}{1 - \epsilon x}, \qquad U = \frac{u}{1 - \epsilon x}, \tag{2.2.15}$$

from Example 2.1.6. Since this group has one parameter, only one equation is necessary to define a *cross-section*. A *cross-section* is given by

$$\mathcal{K}^{(0)} = \{x = 1\},$$

leading to the *normalization equation*

$$X = 1.$$

This implies

$$\frac{x}{1-\epsilon x} = 1 \;\Rightarrow\; \epsilon = \frac{1-x}{x}, \qquad x \neq 0,$$

and it completely defines the moving frame map $\rho^{(n)}$: an application which associates to each $\mathfrak{z}^{(n)} \in \mathcal{J}^{(n)}$ the pseudo-group element which has $\epsilon = \frac{1-x}{x}$.

Using the chain rule, the pseudo-group action on the jet bundle $\mathcal{J}^{(1)}$ with local coordinates $\{s, x, u, x_s, u_s\}$ is found to be

$$\begin{gathered} S = s, \qquad X = \frac{x}{1-\epsilon x}, \qquad U = \frac{u}{1-\epsilon x}, \\ X_s = \frac{x_s}{(1-\epsilon x)^2}, \qquad U_s = \frac{u_s + \epsilon(u\,x_s - u_s\,x)}{(1-\epsilon x)^2}. \end{gathered} \tag{2.2.16}$$

The application of the moving frame map $\rho^{(n)}$ to all local coordinates in $\mathcal{J}^{(1)}$ is obtained by substituting $\epsilon = \frac{1-x}{x}$ into (2.2.16) and it yields a complete set of differential invariants of order $\leq 1$

$$\begin{gathered} \iota(s) = s, \qquad \iota(x) = 1, \qquad \iota(u) = \frac{u}{x}, \\ \iota(x_s) = \frac{x_s}{x^2}, \qquad \iota(u_s) = \frac{u\,x_s - u\,x\,x_s + u_s\,x^2}{x^3}. \end{gathered} \tag{2.2.17}$$

Note that in standard variables, a complete set of invariants is

$$\begin{gathered} \iota(x) = 1, \qquad \iota(u) = \frac{u}{x}, \\ \iota(u_x) = \iota\left(\frac{u_s}{x_s}\right) = \frac{u - x\,u + x^2\,u_x}{x}, \end{gathered}$$

which can be found either by the moving frame approach applied to the standard variables space $\mathrm{J}^{(1)}$ or by using the Lie algebra approach (the infinitesimal generator of the action was given in Example 2.1.13, Equation (2.1.20)). Note that

$$\iota\left(\frac{u_s}{x_s}\right) = \frac{\iota(u_s)}{\iota(x_s)}$$

since $\iota F(\mathfrak{z}^{(n)}) = F(\iota(\mathfrak{z}^{(n)}))$.

In the previous example, the pseudo-group dimension was 1 and this meant that a single *normalization equation* was sufficient to define a moving frame. However, the next example shows that, when there are more parameters, it might be necessary to prolong the action to higher order jets so that it is possible to choose a *cross-section*.

**Example 2.2.14.** Consider the pseudo-group action

$$X = x, \qquad U = \lambda u + \epsilon, \qquad \lambda \geq 1,\ \epsilon \geq 0, \tag{2.2.18}$$

which is a two-dimensional Lie group action belonging to Dorodnitsyn, Kozlov and Winternitz's classification, [**20**], under the name $\mathbf{D_{2,4}}$. Since this group has two parameters, two equations are necessary to define a *cross-section*. However, no *cross-section* in $\mathcal{J}^{(0)}$ enables one to solve *normalization equations* for the two parameters $\lambda$ and $\epsilon$. It is necessary to prolong the action to $\mathcal{J}^{(1)}$ :

$$S = s, \qquad X = x, \qquad U = \lambda u + \epsilon, \qquad X_s = x_s, \qquad U_s = \lambda u_s.$$

A *cross-section* is now given by

$$\mathcal{K}^{(1)} = \{u = 0, u_s = 1\},$$

leading to the *normalization equations*

$$U = 0, \qquad U_s = 1.$$

This implies

$$\lambda = \frac{1}{u_s}, \qquad \epsilon = -\frac{u}{u_s}, \qquad u_s \neq 0.$$

The pseudo-group action on $x_{ss}$ and $u_{ss}$ is

$$X_{ss} = x_{ss}, \qquad U_{ss} = \lambda u_{ss}.$$

Substituting $\lambda = \frac{1}{u_s}$ into the action yields a complete set of differential invariants of order $\leq 2$

$$\begin{gathered} \iota(s) = s, \qquad \iota(x) = x, \qquad \iota(u) = 0, \\ \iota(x_s) = x_s, \qquad \iota(u_s) = 1, \\ \iota(x_{ss}) = x_{ss}, \qquad \iota(u_{ss}) = \frac{u_{ss}}{u_s}, \end{gathered} \tag{2.2.19}$$

All of which are nontrivial invariants except for the constants 0 and 1.

The situation exposed in Example 2.2.14 is typical of $n$-dimensional pseudo-group actions: one hopes that prolonging the action to higher order jets eventually supplies enough dimensions to choose $n$ linearly independent *normalization equations* so that it is possible to solve uniquely for the $n$ parameters.

In both previous examples, the Lie pseudo-groups were finite-dimensional. For infinite-dimensional Lie pseudo-groups, the arbitrary functions appearing in the action and all their derivatives are treated as pseudo-group parameters. Each time the action is prolonged to a higher order, the jet bundle $\mathcal{J}^{(n)}$ grows larger, offering more dimensions to choose a *cross-section* $\mathcal{K}^{(n)}$, but, at the same time, higher order derivatives of the arbitrary functions appear in the prolonged action, i.e. the number of parameters grows with $n$. The next example illustrates this situation.

**Example 2.2.15.** In this example, a complete set of differential invariants of order $\leq 2$ of the pseudo-group

$$X = f(x), \qquad Y = y, \qquad U = \frac{u}{f'(x)}, \tag{2.2.20}$$

is constructed using the computational variables $(s,t)$ so that $x = x(s,t)$, $y = y(s,t)$ and $u = u(s,t)$. The computations in standard variables $(x, y, u(x,y))$ appear in [**54**]. As in Example 2.2.9, let the relations between standard and computational variables be constrained by the equations (2.2.12). The prolongation of this action was computed up to order 1 in Example 2.2.9. The result is reproduced here and completed up to order 2

$$\begin{gathered}
S = s, \qquad T = t, \qquad Y = y, \qquad X = f(x), \qquad U = \frac{u}{f_x}, \\
X_s = f_x\, x_s, \qquad Y_t = k, \qquad U_s = \frac{u_s}{f_x} - \frac{u\, f_{xx}\, x_s}{f_x^2}, \qquad U_t = \frac{u_t}{f_x}, \\
X_{ss} = f_{xx}\, x_s^2 + f_x\, x_{ss}, \qquad Y_{tt} = 0, \qquad U_{tt} = \frac{u_{tt}}{u}, \qquad U_{st} = \frac{u_{st}}{f_x} - \frac{u_t\, f_{xx}\, x_s}{f_x^2}, \\
U_{ss} = \frac{u_{ss}}{f_x} + 2\frac{u\, f_{xx}^2\, x_s^2}{f_x^3} - 2\frac{u_s\, f_{xx}\, x_s}{f_x^2} - \frac{u\, f_{xxx}\, x_s^2}{f_x^2} - \frac{u\, f_{xx}\, x_{ss}}{f_x^2}.
\end{gathered} \tag{2.2.21}$$

The parameters appearing in the second order prolonged action (2.2.21) are $\{f, f_x, f_{xx}, f_{xxx}\}$. Thus, the *cross-section* must at least lead to four *normalization equations*. A good choice is given by

$$\mathcal{K}^{(2)} = \{x = 0,\ u = 1,\ u_s = 0,\ u_{ss} = 0\}. \tag{2.2.22}$$

When solving the *normalization equations*

$$X = 0, \qquad U = 1, \qquad U_s = 0, \qquad U_{ss} = 0,$$

for the pseudo-group parameters $f, f_x, f_{xx}, f_{xxx}$, the right moving frame

$$f = 0, \qquad f_x = u, \qquad f_{xx} = \frac{u_s}{x_s}, \qquad f_{xxx} = \frac{u_{ss}}{x_s^2} - \frac{u_s\, x_{ss}}{x_s^3}, \tag{2.2.23}$$

is obtained. Although this is not a moving frame for the full pseudo-group[3], it is sufficient to find a moving frame for the second order action since only these four

[3] A *cross-section* for the full pseudo-group is given by $\mathcal{K}^{(\infty)} = \{x = 0,\ u = 1,\ u_{s^k} = 0,\ k \geq 1\}$

parameters appear in it. Substituting the pseudo-group parameters (2.2.23) into the prolonged action (2.2.21) yields the differential invariants

$$\begin{gathered}
\iota(s) = s, \qquad \iota(t) = t, \qquad \iota(x) = 0, \qquad \iota(y) = y, \qquad \iota(u) = 1 \\
I_1 = \iota(x_s) = u\, x_s, \qquad \iota(y_t) = k, \qquad \iota(u_s) = 0, \qquad J_{0,1} = \iota(u_t) = \frac{u_t}{u}, \\
I_2 = \iota(x_{ss}) = u_s\, x_s + u\, x_{ss}, \qquad \iota(y_{tt}) = 0, \qquad \iota(u_{ss}) = 0 \\
J_{0,2} = \iota(u_{tt}) = \frac{u_{tt}}{u}, \qquad J_{1,1} = \iota(u_{st}) = \frac{u\, u_{st} - u_t\, u_s}{u^2}.
\end{gathered} \tag{2.2.24}$$

The previous examples were chosen such that moving frames would exist. Unfortunately, this is not always the case. For a moving frame to exist, the pseudo-group action must be *free* and *regular*, [**54**]. These technical requirements are defined for future reference in the following although, in practice, the existence of a moving frame is usually determined by inspection, i.e. by trying to find a *cross-section* and solve the *normalization equations* for the pseudo-group parameters.

**Definition 2.2.16.** A Lie pseudo-group is said to act regularly on $M$ if all the orbits have the same dimension and if each point $x \in M$ has arbitrarily small neighborhoods whose intersection with each orbit is a connected subset.

**Definition 2.2.17.** Let

$$\mathcal{G}^{(n)}_{\mathfrak{z}^{(n)}} = \left\{ g^{(n)} \in \mathcal{G}^{(n)}|_{\mathfrak{z}} \,:\, g^{(n)} \cdot \mathfrak{z}^{(n)} = \mathfrak{z}^{(n)} \right\}$$

denote the *isotropy subgroup* of $\mathfrak{z}^{(n)} \in \mathcal{J}^{(n)}$. The pseudo-group $\mathcal{G}$ is said to act *freely* at $\mathfrak{z}^{(n)} \in \mathcal{J}^{(n)}$ if $\mathcal{G}^{(n)}_{\mathfrak{z}^{(n)}} = \{\mathbb{1}^{(n)}|_{\mathfrak{z}}\}$. The pseudo-group $\mathcal{G}$ is said to act *freely at order n* if it acts freely on an open subset $\mathcal{V}^{(n)} \subset \mathcal{J}^{(n)}$, called the set of *regular n-jets.*

The definition of regularity implies that, locally, it is possible to choose a *cross-section* having a unique intersection with each orbit (see Figure 2.2). Freeness implies that, locally, there is a unique $g^{(n)}$ sending each point $\mathfrak{z}^{(n)}$ to the *cross-section*, or,

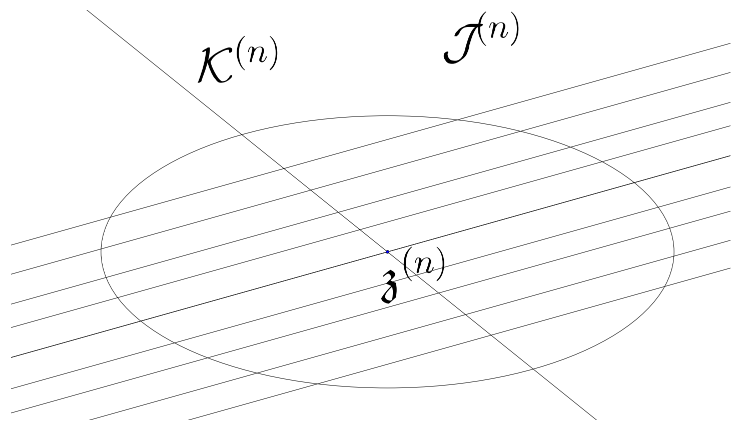


FIG. 2.2. Orbits forming a regular foliation in a neighborhood of $\mathfrak{z}^{(n)}$.

in other words, that there is a unique solution to the system of *normalization equations*. When a pseudo-group action is not free, i.e. when there is more pseudo-group parameters than possible linearly independent *normalization equations*, it is often possible to make it free by prolonging the action to higher order jets so that it is possible to choose the same number of linearly independent *normalization equations* as the number of pseudo-group parameters. For example, in Example 2.2.14, the pseudo-group action was not free on $\mathcal{J}^{(0)}$ but it became free when prolonged to $\mathcal{J}^{(1)}$. The freeness condition can be relaxed but it is not necessary to elaborate on the subject for the purpose of this dissertation.

## 2.3. Discrete invariants

This section explains how to find invariant finite difference approximations of differential invariants using moving frames. The presentation follows Olver's work, [**50**].

Differential invariants being differential functions on the jet bundle $\mathrm{J}^{(n)}$ (or $\mathcal{J}^{(n)}$), it is necessary to first describe how continuous derivatives (which constitute local coordinates in jet bundles) are approximated by finite differences. Before tackling functions of $n$ independent variables, the following lays down some basic principles for functions of 1 and then 2 independent variables.

Consider a smooth function $u = f(x)$ of one variable. Its derivatives $u^{(n)} = f^{(n)}(x)$ are approximated by taking ratios involving differences of the function evaluated at distinct points $u_0 = f(x_0), \ldots, u_k = f(x_k)$ and differences of the independent variables $x_N$, $N \in \{0, \ldots, k\} \subset \mathbb{Z}$. For example, if $x_N = x_0 + Nh$, with $N \in \mathbb{Z}$ and $h$ a constant different from 0, the forward finite differences approximating the first two continuous derivatives of $u$ at $x_N$ are given by

$$\begin{aligned} u_x &\approx \frac{u_{N+1} - u_N}{x_{N+1} - x_N} = \frac{u_{N+1} - u_N}{h}, \\ u_{xx} &\approx \frac{u_{N+2} - 2\,u_{N+1} + u_N}{(x_{N+1} - x_N)^2} = \frac{u_{N+2} - 2\,u_{N+1} + u_N}{h^2}. \end{aligned} \tag{2.3.1}$$

The finite difference approximating $u_{xxx}$ involves a fourth point $(x_{N+3}, u_{N+3})$, the one approximating $u_{xxxx}$ involves a fifth point $(x_{N+4}, u_{N+4})$, and so on. These expressions can be found in almost any introductory textbook on numerical analysis and are essentially derivatives without limit.

Notice the appearance of indices $N \in \mathbb{Z}$ to label discrete points. The index $N$ is a *discrete computational variable* corresponding to a unit length discretization of the computational variable $s$. In this setting, the variables $x$ and $u$ are dependent variables taking values above each index $N \in \mathbb{Z}$. The formulas for the finite differences (2.3.1) depend on the relation between $x$ and the discrete computational variable $N$

which was given here by $x_N = x_0 + Nh$.

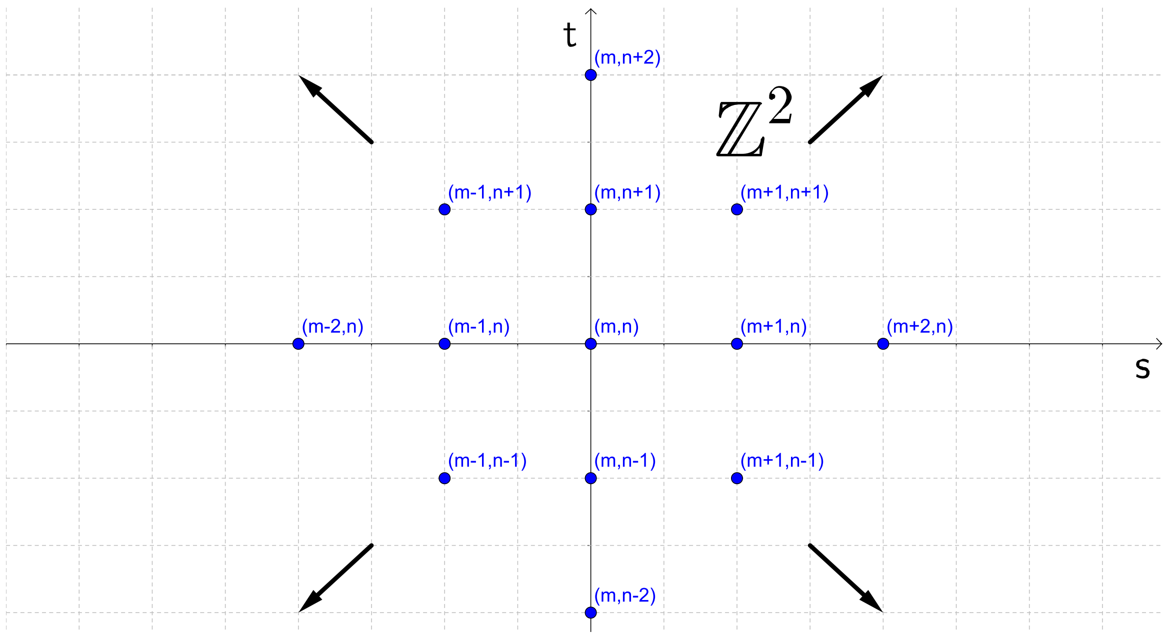


FIG. 2.3. Unit length grid discretization of the two-dimensional computational variables space with coordinates $(s, t)$

Let us now look at finite differences approximating first order partial derivatives of functions $u = f(x, y)$ of two variables. To approximate derivatives in the two independent directions $x$ and $y$, it is necessary to use a set of values $u_N$ living above a two-dimensional space, i.e. $N \in \mathbb{Z}^2$. The space $\mathbb{Z}^2$ should be thought of as a unit length grid discretization of the two-dimensional computational variables space with coordinates $(s, t)$. This grid is displayed in Figure 2.3 where it is centered around the index $N = (m, n)$. Each variable $(x, y, u)$ takes a value above each index $N \in \mathbb{Z}^2$, yielding the points $z_N = (x_N, y_N, u_N)$. The finite difference expressions approximating the partial derivatives depend on the relation between standard and computational variables. The most common choice is to pick

$$x_{m+1,n}-x_{m,n}=h, \qquad x_{m,n+1}-x_{m,n}=0, \qquad y_{m+1,n}-y_{m,n}=0, \qquad y_{m,n+1}-y_{m,n}=k, \tag{2.3.2}$$

with $h, k \in \mathbb{R}$. The relations (2.3.2) define an orthogonal grid in $x$ and $y$ living on top of the computational grid displayed in Figure 2.3. However, the steps in $x$ between two adjacent points on an horizontal line are of length $h$ while the steps in $y$ between two adjencent points on a vertical line are of length $k$. When equations (2.3.2) hold, the first order partial derivatives can be approximated at $N = (m, n)$ by the finite differences

$$u_x \approx \frac{u_{m+1,n}-u_{m,n}}{x_{m+1,n}-x_{m,n}}, \qquad u_y \approx \frac{u_{m,n+1}-u_{m,n}}{y_{m,n+1}-y_{m,n}}.$$

Although the discussion above does not provide an algorithm to find finite differences approximating partial derivatives of any order for functions of several variables (it is partly the subject of Chapter 3), there is a certain number of features which stand out from it. First, for functions $u = f(x) = f(x^1, \ldots, x^p)$ of $p$ independent variables, there are partial derivatives in $p$ independent directions and finite differences approximating these partial derivatives will use points living above a unit length hypercube grid given by $\mathbb{Z}^p$. Each point $z = (x, u) = (x^1, \ldots, x^p, u)$ takes a value above each dot $N \in \mathbb{Z}^p$ of the grid and is labeled accordingly by the multi-index

$$z_N = (x_N, u_N), \qquad N = (n^1, \ldots, n^p) \in \mathbb{Z}^p.$$

Moreover, finite differences approximating continuous derivatives are functions $F(z_{N_1}, \ldots, z_{N_k})$, where $N_i \in \mathbb{Z}^p$, defined on the $k$-fold cartesian product $M^{\times k} = M \times \ldots \times M$, where the number of points $k$ needed depends on the order (and the accuracy) of the derivatives one wishes to approximate. To be more precise, finite differences involve the evaluation of a function at a certain number $k$ of **distinct** points and so we define the following *joint product*.

**Definition 2.3.1.** The $k$-fold *joint product* of a manifold $M$ is a subset of the $k$-fold Cartesian product $M^{\times k}$ given by

$$M^{\diamond k} = \{(z_{N_1}, \dots, z_{N_k}) \,|\, z_{N_i} \neq z_{N_j} \text{ for all } i \neq j\} \subset M^{\times k}.$$

So finite differences are functions defined on the *joint product* $M^{\diamond k}$.

The fiber of the jet bundle $\mathrm{J}^{(n)}$ at a point $z = (x, u)$ is obtained by adding the derivatives of $u$ up to order $n$ such that local coordinates in $\mathrm{J}^{(n)}$ become $z^{(n)} = (x, u^{(n)})$. To define the finite differences approximating the partial derivatives $u^{(n)}$, it is necessary to use more and more points as $n$ grows. The finite differences are thus defined on a joint product $M^{\diamond k}$ where $k$ grows with $n$ since $M^{\diamond k}$ contains the same number of copies of $M$ as the number of points $k$ used to define the finite differences.

**Definition 2.3.2.** The $n^{\text{th}}$ order *forward discrete jet* at the multi-index $N$ is the point

$$\mathfrak{z}_N^{[n]} = (N, \dots\ z_{N+K}\ \dots) \in M^{\diamond d_n}, \tag{2.3.3}$$

where $K \in \mathbb{N}^p$ with $0 \leq \#K \leq n$ and $d_n$ is the number of such multi-indices $K$.

In dimension 2, Figure 2.4 shows the multi-indices contained in a forward discrete jet at the point $\mathfrak{z}_{m,n}^{[k]}$. Geometrically, the multi-indices included in $\mathfrak{z}_{(m,n)}^{[k]}$ are those contained inside and on the boundary of the right isosceles triangle with vertices at $(m, n)$, $(m + k, n)$ and $(m, n + k)$. These multi-indices are other points of $(Z)^p$, neighbors of $N$, which enables one to define discrete derivatives.

Let $\mathcal{J}^{[n]}$ be the space with local coordinates given by forward discrete jets $\mathfrak{z}_N^{[n]}$. The space $\mathcal{J}^{[n]}$ is called the $n^{\text{th}}$ order *forward joint space*.

The following shows that the *forward discrete jets* $\mathfrak{z}_N^{[n]}$, which are local coordinates on $\mathcal{J}^{[n]}$, are a discrete approximation (modulo a change of variables) of the continuous local coordinates $\mathfrak{z}^{(n)}$ on $\mathcal{J}^{(n)}$.

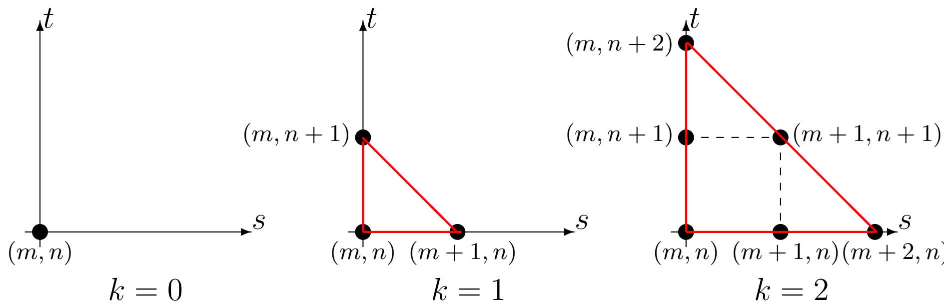


FIG. 2.4. Multi-indices occurring in $\mathfrak{z}_{m,n}^{[k]}$ for $k=0,1,2$.

Let $e^i = (0,\ldots,0,1,0,\ldots,0)$ be the $i^{\text{th}}$ element of the standard orthonormal basis of $\mathbb{R}^p$. Also, let

$$S_i(z_N) = z_{N+e_i}, \qquad i=1,\ldots,p, \tag{2.3.4}$$

denote the usual forward shift operator in the $i^{\text{th}}$ component. Then, on a unit hypercube grid, the derivative operators $D_{s^i}$ can be approximated by the forward difference

$$D_{s^i} \sim \Delta_i = S_i - \mathbb{1}, \qquad i=1,\ldots p, \tag{2.3.5}$$

where $\mathbb{1}(z_N) = z_N$ is the identity map. Then, for a non-negative multi-index $K = (k^1,\ldots,k^p)$,

$$z_{s^K}^N = \Delta_K(z_N) = \Delta_1^{k_1}\cdots\Delta_p^{k_p}(z_N) \tag{2.3.6}$$

is a forward finite difference approximating the derivative $z_{s^K}$ at the point $s=N$.

Making the change of variables $z_{N+K} \mapsto z^N_{s^K}$, we have that local coordinates on $\mathcal{J}^{[n]}$, at the point $s = N$,

$$\mathfrak{z}^{[n]}_N \simeq (N, \ldots\ z^N_{s^K}\ \ldots) = (N, \ldots\ x^N_{s^K} \ldots u^N_{s^K} \ldots), \qquad 0 \leq \#K \leq n, \tag{2.3.7}$$

are a finite difference approximation of local coordinates $\mathfrak{z}^{(n)} = (s, x^{(n)}, u^{(n)})$ of $\mathcal{J}^{(n)}$ at the point $s = N$.

**Remark 2.3.3.** In (2.3.6) and elsewhere, the usual derivative notation is supplemented by a superscript to denote (forward) discrete derivatives. The superscript indicates where the derivative is evaluated.

**Example 2.3.4.** This example illustrates the correspondence between $\mathcal{J}^{[1]}$ and $\mathcal{J}^{(1)}$ for a manifold $M$ with local coordinates $z = (x, y, u(x, y))$. By definition, local coordinates in $\mathcal{J}^{(1)}$ are given by

$$(s, t, z, z_s, z_t) = (s, t, x, y, u, x_s, y_s, u_s, x_t, y_t, u_t).$$

On the other hand, local coordinates in $\mathcal{J}^{[1]}$ at $N = (m, n)$ are given by

$$\begin{aligned} &(m, n, z_{m,n}, z_{m+1,n}, z_{m,n+1}) = \\ &\qquad (m, n, x_{m,n}, y_{m,n}, u_{m,n}, x_{m+1,n}, y_{m+1,n}, u_{m+1,n}, x_{m,n+1}, y_{m,n+1}, u_{m,n+1}). \end{aligned} \tag{2.3.8}$$

Let us apply the change of variables

$$z_{m,n} \mapsto z_{m,n}, \qquad z_{m+1,n} \mapsto z^{m,n}_s = \Delta_1 z_{m,n}, \qquad z_{m,n+1} \mapsto z^{m,n}_t = \Delta_2 z_{m,n},$$

where $\Delta_1 z_{m,n}$ means $(x_{m+1,n} - x_{m,n}, y_{m+1,n} - y_{m,n}, u_{m+1,n} - u_{m,n})$ and similarly in the second component for $\Delta_2 z_{m,n}$. So the new local coordinates in $\mathcal{J}^{[1]}$ are given by $(m, n, z_{m,n}, z^{m,n}_s, z^{m,n}_t)$ which is a finite difference approximation of the continuous local coordinates $(s, t, z, z_s, z_t)$ of $\mathcal{J}^{(1)}$ on a unit square grid in $(s, t)$.

As pointed out just before Definition 2.3.2, prolongations in a discrete space are obtained by adding points (instead of derivatives as in the continuous case). Given a Lie pseudo-group $\mathcal{G}$ acting on a manifold $M$, let $\mathcal{G}^{[n]}$ be the *discrete prolongation* of $\mathcal{G}$ given by copying the action onto each point of the prolonged discrete space such that

$$g_N^{[n]} = (\ldots, g|_{N+K}, \ldots), \qquad 0 \leq \#K \leq n,$$

whenever $g|_{N+K}$ is defined for all $K$. There is an induced *k-fold product* action of $\mathcal{G}^{[n]}$ on $\mathcal{J}^{[n]}$ given by applying the action component wise on the local coordinates given by the discrete jets

$$\mathfrak{Z}_N^{[n]} = g_N^{[n]} \cdot \mathfrak{z}_N^{[n]} = (N, \ldots, g|_{N+K} \cdot z|_{N+K}, \ldots)$$

provided the points $\mathfrak{z}_N^{[n]} \in \operatorname{dom} g_N^{[n]}$. Once again, the computational variables $N$ are unaffected by the action.

**Example 2.3.5.** Let $M$ be a smooth manifold with local coordinates given by $(x, u)$. Consider again the Lie pseudo-group of finite type (2.2.18). Let $(m, x_m, u_m, x_{m+1}, u_{m+1})$ be local coordinates on $\mathcal{J}^{[1]}$. The induced action on $\mathcal{J}^{[1]}$ is given by

$$\begin{gathered} M = m, \qquad X_m = x_m, \qquad U_m = \lambda u_m + \epsilon, \\ X_{m+1} = x_{m+1}, \qquad U_{m+1} = \lambda u_{m+1} + \epsilon, \end{gathered} \tag{2.3.9}$$

which is simply the action (2.2.18) copied to all points and leaving the computational variable unaffected.

Consider now the Lie pseudo-group of infinite type

$$X = f(x), \qquad U = u,$$

where $f \in \mathcal{D}(\mathbb{R})$. The induced action on $\mathcal{J}^{[1]}$ is given by

$$\begin{gathered} M = m, \qquad X_m = f(x_m), \qquad U_m = u_m, \\ X_{m+1} = f(x_{m+1}), \qquad U_{m+1} = u_{m+1}. \end{gathered} \tag{2.3.10}$$

Note that since $f$ is an arbitrary diffeomorphism, $f(x_m)$ and $f(x_{m+1})$ are independent and can be considered as two different parameters. Thus, this simple example is sufficient to outline a fundamental difference between pseudo-groups of finite and infinite types: for finite type pseudo-groups, the number of parameters does not change when the action is prolonged, on the other hand, for infinite type pseudo-groups, each copy of the action on a new point introduces new parameters.

**Definition 2.3.6.** A *discrete* (or *joint*) *invariant* is a function $I : \mathcal{J}^{[n]} \to \mathbb{R}$ which is unaffected by the prolonged action of $\mathcal{G}^{[n]}$ on $\mathcal{J}^{[n]}$, and so

$$I(\mathfrak{Z}_N^{[n]}) = I(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}) = I(\mathfrak{z}_N^{[n]}), \quad \forall \mathfrak{z}_N^{[n]} \in \mathcal{J}^{[n]},\ \forall g_N^{[n]} \in \mathcal{G}^{[n]},$$

where defined.

So the joint space $\mathcal{J}^{[n]}$ plays the same role for discrete invariants as the jet bundle $\mathcal{J}^{(n)}$ plays for differential invariants.

**Example 2.3.7.** The discrete function

$$I(x_m, x_{m+1}, u_m, u_{m+1}) = \frac{u_m\,(x_{m+1} - x_m) + x_m\,(x_m\, u_{m+1} - x_{m+1}\, u_m)}{x_m\,(x_{m+1} - x_m)} \tag{2.3.11}$$

is a discrete invariant of the pseudo-group (2.1.3). The first order prolongation $\mathcal{G}^{[1]}$ of the action (2.1.3) on $\mathcal{J}^{[1]}$, with local coordinates $\{m, z_m, z_{m+1}\}$ and where $z_m = (x_m, u_m)$, is given by

$$M = m, \qquad X_i = \frac{x_i}{1 - \epsilon x_i}, \qquad U_i = \frac{u_i}{1 - \epsilon x_i}, \qquad i = m,\ m+1.$$

This implies

$$
\begin{aligned}
X_{m+1} - X_m &= \frac{x_{m+1}}{1-\epsilon x_{m+1}} - \frac{x_m}{1-\epsilon x_m} \\
&= \frac{x_{m+1}(1-\epsilon x_m) - x_m(1-\epsilon x_{m+1})}{(1-\epsilon x_m)(1-\epsilon x_{m+1})} \\
&= \frac{x_{m+1} - x_m}{(1-\epsilon x_m)(1-\epsilon x_{m+1})}.
\end{aligned}
$$

Thus

$$
\begin{aligned}
I(X_m, X_{m+1}, U_m, U_{m+1}) &= \frac{\dfrac{u_m\,(x_{m+1}-x_m)}{(1-\epsilon x_m)^2(1-\epsilon x_{m+1})} + \dfrac{x_m\,(x_m\,u_{m+1} - x_{m+1}\,u_m)}{(1-\epsilon x_m)^2(1-\epsilon x_{m+1})}}{\dfrac{x_m\,(x_{m+1}-x_m)}{(1-\epsilon x_m)^2(1-\epsilon x_{m+1})}} \\
&= \frac{u_m\,(x_{m+1}-x_m) + x_m\,(x_m\,u_{m+1} - x_{m+1}\,u_m)}{x_m\,(x_{m+1}-x_m)} \\
&= I(x_m, x_{m+1}, u_m, u_{m+1}),
\end{aligned}
$$

and $I$ is a discrete invariant of the pseudo-group (2.1.3).

Moving frames can be used to generate discrete (joint) invariants. To do so, it suffices to replace the continuous jet bundle $\mathcal{J}^{(n)}$ by the joint space $\mathcal{J}^{[n]}$ and invariantize the discrete local coordinates $\mathfrak{z}_N^{[n]}$ instead of the continuous ones.

**Proposition 2.3.8.** The application of the moving frame map to all local coordinates

$$\rho^{(n)}(\mathfrak{z}_N^{[n]}) \cdot \mathfrak{z}_N^{[n]}$$

forms a complete set of discrete (joint) invariants on $d_n$ points, where $d_n$ is defined as in Definition 2.3.2.

As in the continuous case, a moving frame is defined by choosing a *cross-section* $\mathcal{K}^{[n]}$, but the ambient space is now the forward joint space $\mathcal{J}^{[n]}$ with local coordinates

$\mathfrak{z}_N^{[n]}$.

**Remark 2.3.9.** It is ill-advised to send two different independent variables $x_{N_i}$ and $x_{N_j}$, $i \neq j$, to the same constant $c$ since the finite differences containing the difference $x_{N_j} - x_{N_i}$ in their denominator would not be well-defined anymore. Yet, these differences need to be well-defined if one wants to be able to approximate continuous derivatives. Thus, the *normalization equations* $\{\ldots, x_{N_i} = c, \ldots, x_{N_j} = c, \ldots\}$ are to be avoided.

**Example 2.3.10.** Consider again the pseudo-group action (2.1.3) acting on $\mathcal{J}^{[1]}$ with local coordinates $\{m, z_m, z_{m+1}\}$, $z_m = (x_m, u_m)$,

$$M = m, \qquad X_i = \frac{x_i}{1 - \epsilon x_i}, \qquad U_i = \frac{u_i}{1 - \epsilon x_i}, \qquad i = m, m+1.$$

A *cross-section* is given by

$$\mathcal{K}^{[0]} = \{x_m = 1\}.$$

It leads to the *normalization equation*

$$X_m = 1.$$

This implies

$$\frac{x_m}{1 - \epsilon x_m} = 1 \;\Rightarrow\; \epsilon = \frac{1 - x_m}{x_m}.$$

A complete set of discrete invariants on two points (in $\mathcal{J}^{[1]}$) is obtained by setting $\epsilon = \frac{1-x_m}{x_m}$ in the action:

$$\begin{aligned} \iota(x_m) &= 1, \qquad & \iota(x_{m+1}) &= \frac{x_m\, x_{m+1}}{x_m - x_{m+1} + x_m\, x_{m+1}}, \\ \iota(u_m) &= \frac{u_m}{x_m}, \qquad & \iota(u_{m+1}) &= \frac{x_m\, u_{m+1}}{x_m - x_{m+1} + x_m\, x_{m+1}}. \end{aligned} \tag{2.3.12}$$

As in the continuous case, the situation for infinite-dimensional pseudo-groups is more subtle. In this case, prolongation adds arbitrary functions evaluated at new points instead of adding derivatives of arbitrary functions.

**Example 2.3.11.** Consider the pseudo-group (2.2.20) acting on $\mathcal{J}^{[1]}$, with local coordinates $(m, n, z_{m,n}, z_{m+1,n}, z_{m,n+1})$,

$$X_{i,j} = f(x_{i,j}), \qquad Y_{i,j} = y_{i,j}, \qquad U_{i,j} = \frac{u_{i,j}}{f'(x_{i,j})}, \tag{2.3.13}$$

where $(i,j) \in \{(m,n), (m+1,n), (m,n+1)\}$ and where the computational variables are unaffected by the action. The parameters $f$ and $f'$ evaluated at each point are all independent since $f$ is an arbitrary local diffeomorphism. Six *normalization equations* are necessary for these six parameters. A *cross-section* is given by

$$\mathcal{K}^{[1]} = \{x_{m,n} = 1,\ x_{m+1,n} = 2,\ x_{m,n+1} = 3,\ u_{m,n} = u_{m+1,n} = u_{m,n+1} = 1\}. \tag{2.3.14}$$

Solving the *normalization equations*

$$X_{m,n} = 1, \qquad X_{m+1,n} = 2, \qquad X_{m,n+1} = 3, \qquad U_{m,n} = U_{m+1,n} = U_{m,n+1} = 1,$$

for the parameters $\{f_{m,n}, f_{m+1,n}, f_{m,n+1}, f'_{m,n}, f'_{m+1,n}, f'_{m,n+1}\}$, where $f_{m,n} = f(x_{m,n})$, yields the moving frame

$$f_{m,n} = 1, \qquad f_{m+1,n} = 2, \qquad f_{m,n+1} = 3, \qquad f'_{i,j} = u_{i,j},$$

where $(i,j) \in \{(m,n), (m+1,n), (m,n+1)\}$. Replacing the values found for these parameters into the action yields a complete set of discrete invariants on three points:

$$\begin{gathered} \iota(x_{m,n}) = 1, \qquad \iota(x_{m+1,n}) = 2, \qquad \iota(x_{m,n+1}) = 3, \\ \iota(y_{m,n}) = y_{m,n}, \qquad \iota(y_{m+1,n}) = y_{m+1,n}, \qquad \iota(y_{m,n+1}) = y_{m,n+1}, \\ \iota(u_{m,n}) = 1, \qquad \iota(u_{m+1,n}) = 1, \qquad \iota(u_{m,n+1}) = 1. \end{gathered} \tag{2.3.15}$$

It is pretty obvious that this action, prolonged to any number of points, only allows the invariants $y_{i,j}$ and trivial invariants (constants).

## 2.4. Invariant discretizations

The previous two sections showed how to find differential and discrete (joint) invariants of Lie pseudo-groups by acting on the jet bundles $\mathcal{J}^{(n)}$ and $\mathcal{J}^{[n]}$ respectively. The goal is now to construct discrete equations which approximate differential ones while preserving their symmetries.

The starting point is a differential equation

$$\Delta(x, u^{(n)}) = 0, \tag{2.4.1}$$

with symmetry (pseudo-)group $\mathcal{G}$. The differential equation is rewritten in terms of computational variables $s$

$$\Delta(s, x^{(n)}, u^{(n)}) = \Delta(x, u^{(n)}) = 0. \tag{2.4.2a}$$

Equation (2.4.2a) can be supplemented by equations specifying the change of variables between standard and computational variables

$$\widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0. \tag{2.4.2b}$$

These equations are called *companion equations*, [**46**]. A differential equation written in computational variables (2.4.2a) and supplemented with companion equations (2.4.2b) form a system of equations called an *extended system*. For the *extended system* (2.4.2) to have the same solution space as the original equation (2.4.1), the companion equations (2.4.2b) cannot introduce differential constraints in the derivatives $u^{(n)}$. Also, they must respect the non-degeneracy condition (2.2.8).

**Example 2.4.1.** Consider the differential equation

$$u_{xx} = 1. \tag{2.4.3}$$

Equation (2.4.3) can be rewritten in computational variables by using the chain rule and the fact that $(x, u) = (x(s), u(s))$ (as was detailed in Section 2, see Example 2.2.8). The first and second order derivatives in computational variables are

$$u_s = u_x\, x_s, \qquad u_{ss} = u_{xx}\, x_s^2 + u_x\, x_{ss},$$

and thus

$$u_x = \frac{u_s}{x_s}, \qquad u_{xx} = \frac{u_{ss}\, x_s - u_s\, x_{ss}}{x_s^3}.$$

So the differential equation (2.4.3) expressed in computational variables becomes

$$\frac{u_{ss}\, x_s - u_s\, x_{ss}}{x_s^3} = 1. \tag{2.4.4}$$

Equation (2.4.4) can be extended if the relation between $x$ and $s$ is specified. For example, if the *companion equation* $x = e^s$ is chosen, Equation (2.4.4) becomes the *extended system*

$$u_{ss} - u_s = e^{2s}, \qquad x = e^s.$$

In the previous example, there was no pseudo-group action specified, but when there is, the companion equations are required to be invariant under the action considered.

**Definition 2.4.2.** Let $\Delta(x, u^{(n)}) = 0$ be a differential equation invariant under a Lie pseudo-group $\mathcal{G}$ action. An extended system of differential equations $\{\Delta(s, x^{(n)}, u^{(n)}) = 0, \widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0\}$ is said to be $\mathcal{G}$-*compatible* with the $\mathcal{G}$-invariant differential equation $\Delta(x, u^{(n)}) = 0$ if it is invariant under the pseudo-group $\mathcal{G}$:

$$\begin{cases} \Delta(s, g^{(n)} \cdot x^{(n)}, g^{(n)} \cdot u^{(n)}) = 0, \\ \widetilde{\Delta}(s, g^{(n)} \cdot x^{(n)}, g^{(n)} \cdot u^{(n)}) = 0, \end{cases} \qquad \text{whenever} \qquad \begin{cases} \Delta(s, x^{(n)}, u^{(n)}) = 0, \\ \widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0. \end{cases}$$

An example of a $\mathcal{G}$-*compatible* extended system will be constructed in Example 2.4.5.

A numerical scheme for the differential equation (2.4.1), or its extended counterpart (2.4.2), is a set of finite difference equations

$$E(\mathfrak{z}_N^{[n]}) = 0, \qquad \widetilde{E}(\mathfrak{z}_N^{[n]}) = 0,$$

having the property that, in the continuous limit, these equations converge to the extended system (2.4.2):

$$E(\mathfrak{z}_N^{[n]}) \to \Delta(s, x^{(n)}, u^{(n)}), \qquad \widetilde{E}(\mathfrak{z}_N^{[n]}) \to \widetilde{\Delta}(s, x^{(n)}, u^{(n)}). \tag{2.4.5}$$

The *discrete companion equations* $\widetilde{E}(\mathfrak{z}_N^{[n]}) = 0$ can be thought of as mesh equations specifying how the standard independent variables depend on the multi-index $N$.

The continuous limit is obtained by coalescing all the multi-indices $N_i$ of the points $z_{N_i}$ to one of them. To do this, introduce the parameters $\sigma_i$ such that the forward sift operators (2.3.4) become

$$S_i(z_N) = z_{N+\sigma_i\, e_i}, \qquad i = 1, \ldots, p,$$

and the difference operators (2.3.5) become

$$D_{s^i} \sim \Delta_i = \frac{S_i - \mathbb{1}}{\sigma_i}, \qquad i = 1, \ldots p. \tag{2.4.6}$$

Taylor expand each $z_{N_i}$ around $N$, with $z = z_N$,

$$P_n[z_{N_i}, N_i](N) = \sum_{\#J=0}^{n} \frac{\partial^J z\big|_N}{J!}(N_i - N)^J,$$

where

$$\#J = j^1 + \cdots + j^p, \qquad J! = j^1! \cdots j^p!, \qquad (N_i - N)^J = \sigma_1^{j^1} \cdots \sigma_p^{j^p},$$

and

$$\partial^J z\big|_N = \left.\frac{\partial^{\#J} z}{(\partial s^1)^{j^1} \cdots (\partial s^p)^{j^p}}\right|_N$$

and then take the limits $\sigma_i \to 0$.

**Example 2.4.3.** Consider the discrete function on four points

$$I^d = \frac{u_{m+1,n+1}\, u_{m,n} - u_{m+1,n}\, u_{m,n+1}}{u_{m,n}\, u_{m,n+1}\, u_{m+1,n}(x_{m+1,n} - x_{m,n})(y_{m,n+1} - y_{m,n})}.$$

Adding parameters $(\sigma, \tau)$ to the shifts transforms the function to

$$\tilde{I}^d = \frac{u_{m+\sigma,n+\tau}\, u_{m,n} - u_{m+\sigma,n}\, u_{m,n+\tau}}{u_{m,n}\, u_{m,n+\tau}\, u_{m+\sigma,n}(x_{m+\sigma,n} - x_{m,n})(y_{m,n+\tau} - y_{m,n})}.$$

The Taylor expansions around $z_{m,n} = z$ with computational variables $(s, t)$ for the points $z_{N_i}$ are given by

$$\begin{aligned}
z_{m+\sigma,n} &= z + \sigma z_s + \frac{\sigma^2}{2} z_{ss} + \ldots, \\
z_{m,n+\tau} &= z + \tau z_t + \frac{\tau^2}{2} z_{tt} + \ldots, \\
z_{m+\sigma,n+\tau} &= z + \sigma z_s + \tau z_t + \frac{\sigma^2}{2} z_{ss} + \sigma\tau z_{st} + \frac{\tau^2}{2} z_{tt} + \ldots.
\end{aligned}$$

This implies

$$\begin{aligned}
u_{m+\sigma,n+\tau}\, u_{m,n} &= u^2 + u\, u_s\, \sigma + u\, u_t\, \tau + u\, u_{ss}\frac{\sigma^2}{2} + u\, u_{st}\sigma\tau + u\, u_{tt}\frac{\tau^2}{2} + \ldots, \\
u_{m+\sigma,n}\, u_{m,n+\tau} &= u^2 + u\, u_s\, \sigma + u\, u_t\, \tau + u\, u_{ss}\frac{\sigma^2}{2} + u_s\, u_t\, \sigma\tau + u\, u_{tt}\frac{\tau^2}{2} \ldots,
\end{aligned}$$

which in turn implies

$$u_{m+\sigma,n+\tau}\, u_{m,n} - u_{m+\sigma,n}\, u_{m,n+\tau} = u\, u_{st}\, \sigma\tau - u_s\, u_t\, \sigma\tau + \dots .$$

Replacing the Taylor expansions in the discrete function $\tilde{I}^d$ yields

$$\begin{aligned} \tilde{I}^d &= \frac{(u\, u_{st} - u_s\, u_t)\sigma\tau + \dots}{u^3\, x_s\, y_t\, \sigma\tau + \dots}, \\ &= \frac{(u\, u_{st} - u_s\, u_t)}{u^3\, x_s\, y_t} + O(\sigma^2, \tau^2), \end{aligned}$$

which goes to, in the limit $\sigma \to 0$ and $\tau \to 0$,

$$I = \frac{(u\, u_{st} - u_s\, u_t)}{u^3\, x_s\, y_t},$$

the differential invariant found in Example 2.2.4.

**Definition 2.4.4.** A Lie pseudo-group $\mathcal{G}$ is a *symmetry (pseudo-)group* of the numerical scheme $\{E(\mathfrak{z}_N^{[n]}) = 0,\ \widetilde{E}(\mathfrak{z}^{[n]}) = 0\}$ if

$$\begin{cases} E(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}) = 0, \\ \widetilde{E}(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}) = 0, \end{cases} \qquad \text{whenever} \qquad \begin{cases} E(\mathfrak{z}_N^{[n]}) = 0, \\ \widetilde{E}(\mathfrak{z}_N^{[n]}) = 0. \end{cases}$$

If a differential equation and its numerical scheme have the same (pseudo-)group of symmetry, the numerical scheme is said to be an *invariant discretization* of the differential equation.

Let $\mathcal{G}$ be the pseudo-group of symmetry of the differential equation (2.4.1). To construct an *invariant discretization* of this differential equation, the following algorithm can be applied:

- Generate a complete set of differential invariants $\{I_1, \dots, I_l\}$ of $\mathcal{G}$ up to order $n$ by defining a moving frame, i.e. by choosing a cross-section $\mathcal{K}^{(n)} \subset \mathcal{J}^{(n)}$;

- Write a $\mathcal{G}$-compatible *extended system* (2.4.2) for the differential equation (2.4.1) expressed in terms of the invariants found, i.e.
$$\begin{cases} \Delta(s, x^{(n)}, u^{(n)}) = E(s, I_1, \ldots, I_l) = 0, \\ \widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = \widetilde{E}(s, I_1, \ldots, I_l) = 0; \end{cases}$$
- Generate a complete set of discrete invariants $\{I_1^d, \ldots, I_l^d\}$ of $\mathcal{G}$ by defining a moving frame such that the cross-section $\mathcal{K}^{[n]} \subset \mathcal{J}^{[n]}$ goes to $\mathcal{K}^{(n)}$ in the continuous limit and where the discrete invariants are obtained by invariantizing the local coordinates $(N, \ldots x^N_{s^K} \ldots u^N_{s^K})$;
- Write the system
$$\begin{cases} E(N, I_1^d, \ldots, I_l^d) = 0, \\ \widetilde{E}(N, I_1^d, \ldots, I_l^d) = 0, \end{cases}$$
which is an invariant discretization of the differential equation (2.4.1).

The fact that the invariant numerical scheme produced by the algorithm has the right continuous limit is guaranteed by the fact that the cross-section $\mathcal{K}^{(n)}$ is the continuous limit of the cross-section $\mathcal{K}^{[n]}$ and as well by the fact that the local coordinates $(N, \ldots x^N_{s^K} \ldots u^N_{s^K})$ converge to the continuous local coordinates in the continuous limit.

**Example 2.4.5.** In this example, an invariant discretization of the differential equation

$$\frac{u - u\,x + u_x\,x^2}{x} = 1 \tag{2.4.7}$$

is constructed. Equation (2.4.7) is invariant under the pseudo-group action (2.1.3). Recall that a complete set of differential invariants of order $\leq 1$ was found in Example

2.2.13, using the cross-section $\mathcal{K}^{(0)} = \{x = 1\}$,

$$\begin{aligned} \iota(s) = s, \qquad \iota(x) = 1, \qquad I_1 \equiv \iota(u) = \frac{u}{x}, \\ I_2 \equiv \iota(x_s) = \frac{x_s}{x^2}, \qquad I_3 \equiv \iota(u_s) = \frac{u\,x_s - u\,x\,x_s + u_s\,x^2}{x^3}. \end{aligned} \tag{2.4.8}$$

Thus, a $\mathcal{G}$-compatible extended system for Equation (2.4.7) is

$$\frac{I_3}{I_2} = 1, \qquad I_2 = h,$$

or, explicitly,

$$\frac{u\,x_s - u\,x\,x_s + u_s\,x^2}{x\,x_s} = 1, \qquad \frac{x_s}{x^2} = h,$$

where $h$ is a constant controlling the rate of change $x_s$. To see that the first equation is equivalent to (2.4.7), it suffices to use the fact that $u_s = u_x\,x_s$ and to simplify the $x_s$. In the discrete case, the parameter $h$ will control the mesh step length.

Local coordinates on $\mathcal{J}^{[1]}$ are given by $(m, x_m, u_m, x_s^m, u_s^m)$. Recall that $x_s^m = x_{m+1} - x_m$ and $u_s^m = u_{m+1} - u_m$ (see Equation (2.3.6)). The pseudo-group action on $\mathcal{J}^{(1)}$ is thus

$$\begin{aligned} X_m = \frac{x_m}{1 - \epsilon x_m}, \qquad U_m = \frac{u_m}{1 - \epsilon x}, \\ X_s^m = X_{m+1} - X_m = \frac{x_{m+1}}{1 - \epsilon x_{m+1}} - \frac{x_m}{1 - \epsilon x_m} = \frac{x_{m+1} - x_m}{(1 - \epsilon x_{m+1})(1 - \epsilon x_m)}, \\ U_s^m = U_{m+1} - U_m = \frac{u_{m+1}}{1 - \epsilon x_{m+1}} - \frac{u_m}{1 - \epsilon x_m} = \frac{u_{m+1} - u_m + \epsilon(u_m\,x_{m+1} - u_{m+1}\,x_m)}{(1 - \epsilon x_{m+1})(1 - \epsilon x_m)}. \end{aligned} \tag{2.4.9}$$

The joint space counterpart of the cross-section $\mathcal{K}^{(0)} = \{x = 1\}$ is $\mathcal{K}^{[0]} = \{x_m = 1\}$ and solving the normalization equation yields

$$\epsilon = \frac{1 - x_m}{x_m}.$$

Substituting $\epsilon$ into (2.4.9) invariantizes the local coordinates:

$$\iota(x_m) = 1, \qquad I_1^d \equiv \iota(u_m) = \frac{u_m}{x_m},$$
$$I_2^d \equiv \iota(x_s^m) = \frac{x_{m+1} - x_m}{x_m\, x_{m+1} - (x_{m+1} - x_m)},$$
$$I_3^d \equiv \iota(u_s^m) = \frac{u_m(x_{m+1} - x_m) + x_m(u_{m+1}\, x_m - u_m\, x_{m+1})}{x_m(x_m\, x_{m+1} - (x_{m+1} - x_m))}.$$

Finally, the numerical scheme

$$\frac{I_3^d}{I_2^d} = 1, \qquad I_2^d = h,$$

or, explicitly,

$$\frac{u_m(x_{m+1} - x_m) + x_m(u_{m+1}\, x_m - u_m\, x_{m+1})}{x_m(x_{m+1} - x_m)} = 1, \qquad \frac{x_{m+1} - x_m}{x_m\, x_{m+1} - (x_{m+1} - x_m)} = h,$$

is an invariant discretization of the differential equation (2.4.7) with mesh step length controlled by the parameter $h$.

Having only one independent variable, the previous example was pretty straightforward. In fact, computational variables were not even an absolute necessity. However, they become crucial in more than one independent variable and it is the subject investigated in Chapter 3.

Once again the situation is more subtle for infinite type pseudo-groups. Comparing Examples 2.2.15 and 2.3.11, where continuous and discrete invariants were computed for the same infinite type pseudo-group, shows that it is sometimes impossible to produce invariant discretizations for infinite type pseudo-groups: the only discrete invariants are functions of the independent variables $y_{i,j}$ while some of the differential invariants are functions of the dependent variable $u$ and its derivatives. To remedy this situation, Chapter 4 introduces a new object called *discretized pseudo-groups* which makes it possible to apply the invariant discretization algorithm explained in this section to infinite type pseudo-groups.

# Chapter 3

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## Symmetry Preserving Numerical Schemes for Partial Differential Equations and their Numerical Tests

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## 3.1. Abstract

The method of equivariant moving frames is used to construct symmetry preserving finite difference schemes of partial differential equations invariant under finite-dimensional symmetry groups. Invariant numerical schemes for a heat equation with logarithmic source and the spherical Burgers' equation are obtained. Numerical tests show how invariant schemes can be more accurate than standard discretizations.

## 3.2. Introduction

In modern numerical analysis, much effort has been invested into developing geometric integrators that incorporate geometrical structures of the system of differential equations being approximated. Well-known examples include symplectic integrators [**13**], energy preserving methods [**61**], Lie–Poisson preserving methods [**71**], and symmetry preserving numerical schemes [**8, 40, 69**]. The motivation behind all this work is that, as a rule of thumb, geometric integrators give better results than many other standard numerical methods since they take into account qualitative properties of the system being studied.

For ordinary differential equations, the problem of generating invariant numerical schemes preserving the point symmetries of the original equations is now well understood [**7, 8, 33, 62**]. There exists two different methods for generating invariant finite difference schemes of differential equations. The first approach, mainly developed by Dorodnitsyn, Levi and Winternitz, is based on Lie's infinitesimal symmetry method [**6, 18, 19, 22, 20, 40, 69**]. This approach makes use of Lie's infinitesimal symmetry criterion [**48**] to obtain finite difference invariants from which an invariant scheme is constructed by finding a combination of the invariants that converges, in the continuous limit, to the original system of differential equations. The second approach, developed by Olver and Kim, consists of using the method of equivariant moving frames [31, 32, 50]. With Lie's infinitesimal method, the construction of invariant schemes can sometimes require a lot of work and insights, on the other hand, with the moving frame method the construction is completely algorithmic. In both cases, the methods have proven their efficiency in generating invariant numerical schemes for ordinary differential equations. In comparison, fewer applications involving partial differential equations can be found in the literature [6, 18, 19, 32, 69].

In this paper we use the equivariant moving frame method to generate invariant finite difference schemes of partial differential equations admitting a finite-dimensional symmetry group. To implement the moving frame method, the first step is to obtain appropriate approximations of the partial derivatives on an arbitrary mesh. In [53], Olver proposes a new approach to the theory of interpolation of functions of several variables, based on non-commutative quasi-determinants, to obtain these approximations. We show here that one can use standard Taylor polynomial approximations to achieve the same goal in a somewhat simpler way. The formulas obtained suggest an interesting interpretation of the continuous limit of the finite difference derivatives. More details are given in Section 3.4.

The paper is structured as follows. In Section 3.3, we introduce the basic theory of invariant numerical schemes of differential equations. The formulas used to approximate derivatives on an arbitrary mesh are introduced in Section 3.4, and with these in hand, we review the multi-moving frame construction in Section 3.5. As with the standard moving frame method, the equivariant multi-frame construction relies on Cartan's normalization of the group parameters. Given a multi-frame, there is a canonical invariantization map which projects finite difference expressions onto their invariant finite difference counterparts. In particular, the invariantization of the finite difference derivatives gives finite difference invariants which, in the continuous limit, converge to the normalized differential invariants [27]. Thus, by rewriting a system of partial differential equations in terms of the normalized differential invariants, an invariant numerical scheme is obtained by replacing the normalized differential invariants by their invariant finite difference approximations. The method is illustrated in Section 5 where invariant numerical schemes are obtained for a heat equation with a logarithmic source and for the spherical Burgers' equation. Section 6 is dedicated to numerical tests in which the precision of our invariant schemes is compared to standard numerical schemes.

## 3.3. Differential Equations and Numerical Schemes

Let $M$ be an $m$-dimensional manifold. For $0 \leq n \leq \infty$, let $\mathrm{J}^n = \mathrm{J}^n(M,p)$ denote the *extended* $n^{th}$ *order jet space* of $1 \leq p < m$ dimensional submanifolds $S \subset M$. The jet space is defined as the space of equivalence classes of submanifolds under the equivalence relation of $n^{\mathrm{th}}$ order contact at a point [**48**]. Given a submanifold $S \subset M$, we introduce the local coordinates $z = (x,u) = (x^1,\ldots,x^p,u^1,\ldots,u^q)$, with $q = m-p$, so that $S$ is locally the graph of a function $f(x)$: $S = \{(x, f(x))\}$. In this coordinate chart the coordinates of an $n$-jet of $S$ are $z^{(n)} = (x, u^{(n)})$, where $u^{(n)}$ denotes the collection of derivatives $u^\alpha_J = \partial^k u^\alpha/(\partial x)^J$ with $0 \leq k = \#J \leq n$.

The approximation of the $n$-jet of a submanifold by finite difference derivatives is based on the evaluation of the submanifold at several points. For reasons which will become clearer in the next section, we label the sample points with a multi-index $z_N = (x_N, u_N) = (x_N, f(x_N))$ where $N = (n^1,\ldots,n^p) \in \mathbb{Z}^p$. For the finite difference derivatives to be well defined, the sample points must be distinct in the independent variables. For this, we introduce the $k$-fold *joint product*

$$M^{\diamond k} = \{(z_{N_1},\ldots,z_{N_k}) |\, x_{N_i} \neq x_{N_j} \text{ for all } i \neq j\}$$

which is a subset of the $k$-fold Cartesian product $M^{\times k}$.

A smooth function $\Delta\colon \mathrm{J}^n \to \mathbb{R}$ on (an open subset of) the $n^{\mathrm{th}}$ order jet space is called a *differential function*, and a system of differential equations is defined by the vanishing of one or more differential functions. In the local coordinates $z^{(n)} = (x, u^{(n)})$ a system of differential equations is given by

$$\Delta_1(x, u^{(n)}) = \cdots = \Delta_\ell(x, u^{(n)}) = 0. \tag{3.3.1}$$

**Definition 3.3.1.** Let $\Delta_\nu(x, u^{(n)}) = 0$, $\nu = 1, \ldots, \ell$, be a system of differential equations. A *finite difference numerical scheme* is a system of equations

$$E_\mu(z_{N_1}, \ldots, z_{N_k}) = 0, \qquad \mu = 1, \ldots, \ell, \ldots, \ell + l,$$

defined on the joint product $M^{\diamond k}$ with the property that in the coalescent limit (continuous limit) $z_{N_i} \to z$, $E_\mu(z_{N_1}, \ldots, z_{N_k}) \to \Delta_\nu(x, u^{(n)})$ for $\mu = 1, \ldots, \ell$ and $E_\mu \to 0$ for $\mu = \ell+1, \ldots, \ell+l$. The role of the last $l$ equations $E_{\ell+1} = 0, \ldots, E_{\ell+l} = 0$ is to impose constraints on the mesh.

There are two restrictions on the equations $E_{\ell+1} = 0, \ldots, E_{\ell+l} = 0$. Firstly, the equations must be compatible so that, provided appropriate initial conditions, the independent variables $x_{N_i}$ are uniquely defined. Secondly, these equations should not impose any restriction on the dependent variables $u_{N_i}$. When these two conditions are satisfied we say that the mesh equations are *compatible*.

In Definition 3.3.1, the number of copies $k$ in the joint product will depend on the order of approximation of the numerical scheme. The minimal number of sample points required to approximate the $n^{\text{th}}$ order system of differential equations (3.3.1) is $k = q\binom{p+n}{n} = \dim \mathrm{J}^n - p$, but more sample points can be added for better numerical precision.

**Example 3.3.2.** A standard numerical scheme for the heat equation

$$\Delta(x, t, u^{(2)}) = u_t - u_{xx} - u \ln u = 0 \tag{3.3.2}$$

with logarithmic source on the uniform rectangular mesh

$$x_{m,n} = h\,m + x_0, \qquad t_{m,n} = k\,n + t_0, \qquad \text{where} \qquad h, k, x_0, t_0 \qquad \text{are constants} \tag{3.3.3}$$

and $m$, $n$ are integers, is given by

$$E_1 = \Delta_t u - \Delta_x^2 u - u_{m,n} \ln u_{m,n} = 0, \tag{3.3.4a}$$

where

$$\Delta_t u = \frac{u_{m,n+1} - u_{m,n}}{k}, \qquad \Delta_x^2 u = \frac{u_{m+2,n} - 2u_{m+1,n} + u_{m,n}}{h^2}$$

are the standard finite difference derivatives on the uniform rectangular lattice (3.3.3). In terms of Definition 3.3.1, the mesh (3.3.3) is defined by the equations

$$E_{2,3,4,5} = \begin{cases} x_{m+1,n} - x_{m,n} = h, & x_{m,n+1} - x_{m,n} = 0, \\ t_{m+1,n} - t_{m,n} = 0, & t_{m,n+1} - t_{m,n} = k. \end{cases} \tag{3.3.4b}$$

Given the initial conditions $x_0$, $t_0$ the equations (3.3.4b) uniquely specify the points $(x_{m,n}, t_{m,n})$.

Now, let $G$ be an $r$-dimensional Lie group acting regularly on $M$. Throughout the paper, we will consistently use lower case letters to denote the source coordinates of the action, and capital letters to denote the target coordinates:

$$X^i = g \cdot x^i, \qquad U^\alpha = g \cdot u^\alpha, \qquad i = 1, \ldots, p, \quad \alpha = 1, \ldots, q, \qquad g \in G. \tag{3.3.5}$$

Since a Lie group action preserves the contact equivalence of submanifolds, it induces an action on $\mathrm{J}^n$:

$$g \cdot z^{(n)} = (g \cdot z)^{(n)}, \qquad g \in G, \tag{3.3.6}$$

called the $n^{\text{th}}$ order prolonged action. In applications, the prolonged action (3.3.6) is obtained by implementing the chain rule. In local coordinates, we use the notation $(X, U^{(n)}) = g \cdot (x, u^{(n)})$ to denote the prolonged action. The Lie group $G$ also induces a natural action on the $k$-fold Cartesian product $M^{\times k}$ given by the product action $G^{\times k}$:

$$g \cdot (z_{N_1}, \ldots, z_{N_k}) = (g \cdot z_{N_1}, \ldots, g \cdot z_{N_k}). \tag{3.3.7}$$

**Definition 3.3.3.** Let $G$ be a Lie group acting regularly on $M \simeq X \times U$ and $\Delta_\nu(x, u^{(n)}) = 0$ a system of differential equations. The system of differential equations is said to be *$G$-invariant* if $\Delta_\nu(g \cdot (x, u^{(n)})) = \Delta_\nu(x, u^{(n)})$ for all $g \in G$. Similarly, let $E_\mu(z_{N_1}, \ldots, z_{N_k}) = 0$ be a system of finite difference equations. Then it is $G$-invariant if $E_\mu(g \cdot (z_{N_1}, \ldots, z_{N_k})) = E_\mu(z_{N_1}, \ldots, z_{N_k})$ for all $g \in G$.

**Remark 3.3.4.** Definition 3.3.3 is slightly restrictive. The general notion of $G$-invariance only requires the symmetry group to map solutions to solutions so that

$$\Delta_\nu(g \cdot (x, u^{(n)})) = 0 \qquad \text{whenever} \qquad \Delta_\nu(x, u^{(n)}) = 0,$$

and similarly for finite difference equations. In the following, we assume the differential equations satisfy the $G$-invariance Definition 3.3.3 so that they can be re-expressed in terms of differential invariants. On the other hand, in order to construct invariant numerical schemes we will allow the mesh equations to be $G$-invariant only on their solution space.

**Example 3.3.5.** The heat equation with logarithmic source (3.3.2) is invariant under the group of transformations

$$X = x + 2\lambda_3 e^t + \lambda_2, \qquad T = t + \lambda_1, \qquad \ln U = \ln u - \lambda_3 e^t x - \lambda_3^2 e^{2t} + \lambda_4 e^t, \tag{3.3.8}$$

where $\lambda_1, \ldots, \lambda_4 \in \mathbb{R}$, [**48**]. By direct computation, it is not difficult to see that the numerical scheme (3.3.4a), on the rectangular mesh (3.3.4b), is only invariant under the 3-dimensional group of transformations

$$X = x + \lambda_2, \qquad T = t + \lambda_1, \qquad \ln U = \ln u + \lambda_4 e^t.$$

To see that the one-parameter group

$$X = x + 2\lambda_3 e^t, \qquad T = t, \qquad \ln U = \ln u - \lambda_3 e^t x - \lambda_3^2 e^{2t}$$

is not a symmetry, it suffices to note that

$$\begin{aligned} X_{m,n+1} - X_{m,n} =& 2\lambda_3(e^{t_{m,n+1}} - e^{t_{m,n}}) + (x_{m,n+1} - x_{m,n}) \\ =& 2\lambda_3(e^{t_{m,n+1}} - e^{t_{m,n}}) \neq 0 \qquad \text{when} \qquad \lambda_3 \neq 0. \end{aligned}$$

As Example 3.3.5 shows, for a numerical scheme to preserve the whole symmetry group of a differential equation, a rectangular mesh might be too restrictive. Consequently, the theory of invariant numerical schemes must be developed over arbitrary meshes.

## 3.4. Finite Difference Derivatives

In this section we obtain finite difference derivative expressions on an arbitrary mesh. There are different ways to do so. One can use the theory of multivariate interpolation [**53**], but we prefer to use Taylor polynomial approximations. Depending on the method used, the expressions for the finite difference derivatives can be slightly different, but this difference does not alter the implementation of the moving frame construction discussed in the next section.

To simplify the notation, we assume that the generic point under consideration corresponds to the zero multi-index. Also, let

$$e_i = (0, \ldots, 0, 1, 0, \ldots, 0), \qquad i = 1, \ldots, p,$$

be the multi-index of length $p$ with 1 in the $i^{\text{th}}$ component, and zero elsewhere. Finally, let

$$\Delta_i z_0 = z_{0+e_i} - z_0 = z_{e_i} - z_0, \qquad i = 1, \ldots, p,$$

be the usual forward difference operator in the $i^{\text{th}}$ component.

To obtain finite difference approximations for the first order derivatives $u^\alpha_{x^i}$ we consider the first order Taylor polynomial expansions

$$\Delta_i u_0^\alpha \approx \sum_{j=1}^{p} \Delta_i x_0^j \cdot u^\alpha_{x^j}, \qquad i = 1, \dots, p, \quad \alpha = 1, \dots, q. \tag{3.4.1}$$

Solving for the first order partial derivatives $u^\alpha_{x^i}$ we obtain

$$\begin{pmatrix} u^\alpha_{x^1} \\ \vdots \\ u^\alpha_{x^p} \end{pmatrix} \approx \begin{pmatrix} u^{\alpha,d}_{x^1} \\ \vdots \\ u^{\alpha,d}_{x^p} \end{pmatrix} = \underbrace{\begin{pmatrix} \Delta_1 x_0^1 & \cdots & \Delta_1 x_0^p \\ \vdots & \ddots & \vdots \\ \Delta_p x_0^1 & \cdots & \Delta_p x_0^p \end{pmatrix}^{-1}}_{\Delta x_0^{-1}} \begin{pmatrix} \Delta_1 u_0^\alpha \\ \vdots \\ \Delta_p u_0^\alpha \end{pmatrix}, \qquad \alpha = 1, \dots, q, \tag{3.4.2}$$

which are well defined provided the matrix $\Delta x_0$ is invertible. When this is the case, the expressions (3.4.2) define first order finite difference derivatives on an arbitrary mesh. To obtain finite difference approximations for the second order derivatives, it suffices to consider the second order Taylor polynomial expansions

$$\begin{aligned} \Delta_j \Delta_i u_0^\alpha \approx \sum_{k=1}^{p} \Delta_j \Delta_i x_0^k \cdot u^\alpha_{x^k} + \sum_{k,l=1}^{p} \big[ & (x^k_{e_i+e_j} - x_0^k)(x^l_{e_i+e_j} - x_0^l) \\ & - \Delta_j x_0^k \cdot \Delta_j x_0^l - \Delta_i x_0^k \cdot \Delta_i x_0^l \big] \frac{u^\alpha_{x^k x^l}}{2}, \end{aligned} \tag{3.4.3}$$

with $1 \leq j \leq i \leq p$ and $\alpha = 1, \dots, q$. Substituting the first order finite difference derivatives (3.4.2) in (3.4.3) and solving for the second order derivatives $u^\alpha_{x^k x^l}$ gives finite difference approximations for second order derivatives. Those are well defined expressions provided that the matrix with coefficients given by the factors in front of the second order derivatives in (3.4.3) is invertible. Continuing in this fashion, it is possible to obtain finite difference approximations for third order derivatives and so on.

We now consider the continuous limit of those finite difference derivative expressions and verify that they converge to the corresponding partial derivatives. The standard way of taking the continuous limit of finite difference quantities is to assume that all nodes $z_{N_i}$ coalesce to the same point $z$, and the role of the multi-index $N_i$ is simply to label the points. In the following, we give a more important role to the multi-index $N_i$. Instead of viewing the solution of a system of partial differential equations (3.3.1) as the graph of a function $(x, u(x))$, we can view a solution as a parametrized $p$-dimensional submanifold

$$S \to M \simeq X \times U, \qquad s = (s^1, \ldots, s^p) \mapsto z(s) = (x(s), u(s))$$

transversed to the fibers $\{c\} \times U$. In this setting, the distinction between the independent variables $x^i$ and the dependent variables $u^\alpha$ disappears. Moving to the finite difference picture, we now view the multi-indices $N_i$ as forming a square grid with edges of length 1 in the parameter space $S$. Then, a point $z_{N_i} \in M$ is just the image of $z(s)$ at $s = N_i$, see Figure 3.1.

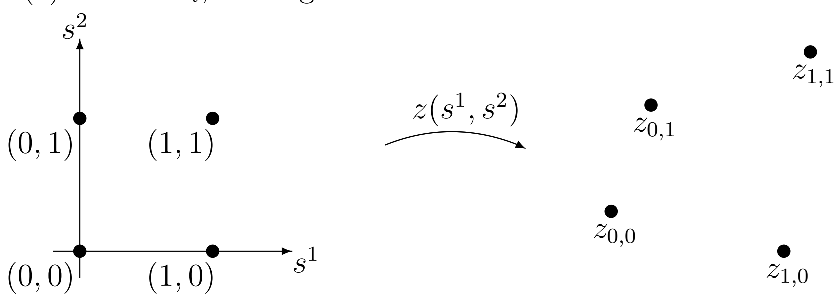



FIG. 3.1. Multi-index interpretation (two independent variables).

In the continuous limit, the point $z_{N_i} = z(N_i)$ converges to $z_0 = z(0) = z$ by coalescing the multi-index $N_i$ to the origin. With this point of view the differences $z_{e_i} - z_0$ converge to $z_{s^i}$ since

$$\Delta_i z_0 = z_{e_i} - z_0 = \left.\frac{z_{\sigma^i e_i} - z_0}{\sigma^i}\right|_{\sigma^i = 1} \xrightarrow{\sigma^i \to 0} z_{s^i}|_z, \qquad i = 1, \ldots, p.$$

Similarly, in the continuous limit

$$\Delta_i \Delta_j z_0 \longrightarrow z_{s^i s^j}|_z, \qquad i, j = 1, \ldots, p,$$

and so on. It thus follows that the expressions (3.4.1) converge to

$$u^\alpha_{s^i} = \sum_{j=1}^{p} x^j_{s^i} \cdot u^\alpha_{x^j}, \qquad \alpha = 1, \ldots, q, \quad i = 1, \ldots, p,$$

which is the chain rule formula for $u = u(x(s))$. Similarly, the expressions (3.4.3) converge to

$$u^\alpha_{s^i s^j} = \sum_{k=1}^{p} x^k_{s^i s^j} u^\alpha_{x^k} + \sum_{k,l=1}^{p} x^k_{s^i} x^l_{s^j} u^\alpha_{x^k x^l}, \tag{3.4.4}$$

in the continuous limit.

**Example 3.4.1.** The above discussion is now specialized to the particular situation of two independent variables $(x, y)$ and one dependent variable $u = u(x, y)$. Without loss of generality, all expressions are centered around $z_{0,0} = (x_{0,0}, y_{0,0}, u_{0,0})$, and neighboring points are denoted by

$$z_{m,n} = (x_{m,n}, y_{m,n}, u_{m,n}), \qquad m, n \in \mathbb{Z}.$$

Also, let

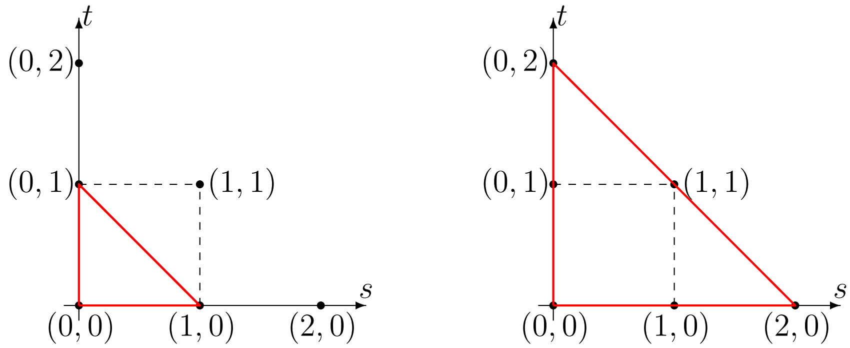
$$\Delta z_{m,n} = z_{m+1,n} - z_{m,n}, \qquad \delta z_{m,n} = z_{m,n+1} - z_{m,n}, \tag{3.4.5}$$

denote the standard forward difference operators in the two indices and let $(s^1, s^2) = (s, t)$ be coordinates for the parameter space $S$.

The indices involved in the expressions of the first and second order discrete partial derivatives are displayed in Figure 2. In general, the definition of the $n^{\text{th}}$ order discrete derivatives will involve the indices contained in the right triangle formed by the origin and the vertices $(n, 0)$, $(0, n)$.

Following our general procedure, to obtain the first order finite difference approximations of $u_x$ and $u_y$ on an arbitrary mesh, the two Taylor expansions

$$u_s \approx \Delta u_{0,0} \approx \Delta x_{0,0} \cdot u_x + \Delta y_{0,0} \cdot u_y, \qquad u_t \approx \delta u_{0,0} \approx \delta x_{0,0} \cdot u_x + \delta y_{0,0} \cdot u_y$$




(a) First order derivatives

(b) Second order derivatives

FIG. 3.2. Indices used to define first and second order discrete partial derivatives.

are considered. Solving for $u_x$ and $u_y$ we obtain

$$u_x \approx u_x^d = \frac{\delta y_{0,0} \cdot \Delta u_{0,0} - \Delta y_{0,0} \cdot \delta u_{0,0}}{\Delta x_{0,0} \cdot \delta y_{0,0} - \delta x_{0,0} \cdot \Delta y_{0,0}}, \qquad u_y \approx u_y^d = \frac{\Delta x_{0,0} \cdot \delta u_{0,0} - \delta x_{0,0} \cdot \Delta u_{0,0}}{\Delta x_{0,0} \cdot \delta y_{0,0} - \delta x_{0,0} \cdot \Delta y_{0,0}}. \tag{3.4.6}$$

In the continuous limit the expressions (3.4.6) converge to

$$u_x = \frac{y_t u_s - y_s u_t}{x_s y_t - x_t y_s}, \qquad u_y = \frac{x_s u_t - x_t u_s}{x_s y_t - x_t y_s}, \tag{3.4.7}$$

which are the usual formulas obtained by the chain rule if $x = x(s,t)$, $y = y(s,t)$.

To obtain approximations for the second order derivatives, it suffices to consider the second order Taylor expansions

$$
\begin{aligned}
u_{ss} \approx \Delta^2 u_{0,0} &\approx \Delta^2 x_{0,0} \cdot u_x + \Delta^2 y_{0,0} \cdot u_y + [(x_{2,0} - x_{0,0})^2 - 2(\Delta x_{0,0})^2]\frac{u_{xx}}{2} \\
&+ [(x_{2,0} - x_{0,0})(y_{2,0} - y_{0,0}) - 2\Delta x_{0,0} \cdot \Delta y_{0,0}]u_{xy} \\
&+ [(y_{2,0} - y_{0,0})^2 - 2(\Delta y_{0,0})^2]\frac{u_{yy}}{2}, \\
u_{st} \approx \delta\Delta u_{0,0} &\approx \delta\Delta x_{0,0} \cdot u_x + \delta\Delta y_{0,0} \cdot u_y + [(x_{1,1} - x_{0,0})^2 - (\Delta x_{0,0})^2 - (\delta x_{0,0})^2]\frac{u_{xx}}{2} \\
&+ [(x_{1,1} - x_{0,0})(y_{1,1} - y_{0,0}) - \Delta x_{0,0} \cdot \Delta y_{0,0} - \delta x_{0,0} \cdot \delta y_{0,0}]u_{xy} \qquad (3.4.8) \\
&+ [(y_{1,1} - y_{0,0})^2 - (\Delta y_{0,0})^2 - (\delta y_{0,0})^2]\frac{u_{yy}}{2}, \\
u_{tt} \approx \delta^2 u_{0,0} &\approx \delta^2 x_{0,0} \cdot u_x + \delta^2 y_{0,0} \cdot u_y + [(x_{0,2} - x_{0,0})^2 - 2(\delta x_{0,0})^2]\frac{u_{xx}}{2} \\
&+ [(x_{0,2} - x_{0,0})(y_{0,2} - y_{0,0}) - 2\delta x_{0,0} \cdot \delta y_{0,0}]u_{xy} \\
&+ [(y_{0,2} - y_{0,0})^2 - 2(\delta y_{0,0})^2]\frac{u_{yy}}{2}.
\end{aligned}
$$

Solving for the second order derivatives $u_{xx}$, $u_{xy}$, $u_{yy}$ in (3.4.8), and replacing the first order derivatives $u_x$, $u_y$ with the approximations (3.4.6), the expressions for the discrete second order derivatives are

$$
\begin{pmatrix} u_{xx} \\ u_{xy} \\ u_{yy} \end{pmatrix} \approx \begin{pmatrix} u^d_{xx} \\ u^d_{xy} \\ u^d_{yy} \end{pmatrix} = H^{-1}V, \tag{3.4.9}
$$

where $V$ is the column vector

$$
V = \begin{pmatrix} \Delta^2 u_{0,0} - \Delta^2 x_{0,0} \cdot u^d_x - \Delta^2 y_{0,0} \cdot u^d_y \\ \delta\Delta u_{0,0} - \delta\Delta x_{0,0} \cdot u^d_x - \delta\Delta y_{0,0} \cdot u^d_y \\ \delta^2 u_{0,0} - \delta^2 x_{0,0} \cdot u^d_x - \delta^2 y_{0,0} \cdot u^d_y \end{pmatrix},
$$

and $H$ is the $3 \times 3$ matrix with entries

$$H_{11} = [(x_{2,0} - x_{0,0})^2 - 2(\Delta x_{0,0})^2]/2, \qquad H_{1,2} = (x_{2,0} - x_{0,0})(y_{2,0} - y_{0,0}) - 2\Delta x_{0,0} \cdot \Delta y_{0,0},$$

$$H_{1,3} = [(y_{2,0} - y_{0,0})^2 - 2(\Delta y_{0,0})^2]/2, \qquad H_{2,1} = [(x_{1,1} - x_{0,0})^2 - (\Delta x_{0,0})^2 - (\delta x_{0,0})^2]/2,$$

$$H_{3,3} = [(y_{0,2} - y_{0,0})^2 - 2(\delta y_{0,0})^2]/2, \qquad H_{2,3} = [(y_{1,1} - y_{0,0})^2 - (\Delta y_{0,0})^2 - (\delta y_{0,0})^2]/2,$$

$$H_{3,1} = [(x_{0,2} - x_{0,0})^2 - 2(\delta x_{0,0})^2]/2, \qquad H_{3,2} = (x_{0,2} - x_{0,0})(y_{0,2} - y_{0,0}) - 2\delta x_{0,0} \cdot \delta y_{0,0},$$

$$H_{2,2} = (x_{1,1} - x_{0,0})(y_{1,1} - y_{0,0}) - \Delta x_{0,0} \cdot \Delta y_{0,0} - \delta x_{0,0} \cdot \delta y_{0,0}.$$

Continuing in this fashion, it is possible to obtain higher order finite difference derivatives on an arbitrary mesh.

The finite difference derivatives constructed above are first order approximations of the continuous derivatives. More accurate approximations can be obtained by using more nodes to approximate the derivatives. Also, the above approximations are constructed solely with the forward difference operators $\Delta_i$. To obtain centered difference approximations one can use the backward and forward difference operators

$$\Delta_i^{\pm} z_{N_l} = \pm(z_{N_l \pm e_i} - z_{N_l}).$$

## 3.5. Equivariant Moving Frames

In this section we review the moving frame construction. The exposition follows [**50**].

**Definition 3.5.1.** Let $G$ be a finite-dimensional Lie group acting smoothly on an $m$-dimensional manifold $M$. A *right moving frame* is a smooth $G$-equivariant map $\rho \colon M \to G$ such that

$$\rho(g \cdot z) = \rho(z) \cdot g^{-1} \qquad \text{for all} \qquad z \in M, \quad g \in G.$$

**Theorem 3.5.2.** A right moving frame exists in a neighborhood of a point $z \in M$ if and only if $G$ acts freely and regularly near $z$.

The action is free if at every point $z \in M$ the isotropy subgroup $G_z = \{e\}$ is trivial. Under this assumption, the group orbits are of dimension $r = \dim G$. The action is regular if the orbits form a regular foliation. The moving frame construction follows from the following theorem.

**Theorem 3.5.3.** If $G$ acts freely and regularly on $M$, and $\mathcal{K} \subset M$ is a cross-section to the group orbits, then the right moving frame $\rho\colon M \to G$ at $z \in M$ is defined as the unique group element $g = \rho(z)$ which sends $z$ to the cross-section $\rho(z) \cdot z \in \mathcal{K}$.

While it is not necessary, we assume $\mathcal{K} = \{z^1 = c^1, \ldots, z^r = c^r\}$ is a coordinate cross-section obtained by fixing the first $r$ components of $z = (z^1, \ldots, z^m)$ to some suitable constants. The moving frame $\rho(z)$ is then obtained by solving the *normalization equations*

$$Z^1 = g \cdot z^1 = c^1, \qquad \ldots \qquad Z^r = g \cdot z^r = c^r, \tag{3.5.1}$$

for the group parameters $g = (g_1, \ldots, g_r)$ in terms of $z = (z^1, \ldots, z^m)$. Given a moving frame, there is a systematic way of associating an invariant to a function.

**Definition 3.5.4.** Let $\rho$ be a right moving frame, the *invariantization* of a scalar function $F\colon M \to \mathbb{R}$ is the invariant function

$$I(z) = \iota(F)(z) = F(\rho(z) \cdot z). \tag{3.5.2}$$

**Proposition 3.5.5.** The invariantization of the coordinate functions $\iota(z^{r+1}), \ldots, \iota(z^m)$ provides a complete set of $m - r$ functionally independent invariants on $M$.

Note that by the moving frame construction, the invariantization of the coordinates defining the normalization equations (3.5.1) are constant, $\iota(z^1) = c^1$, …, $\iota(z^r) = c^r$. Also, if $I(z)$ is an invariant then $\iota(I) = I$.

For most groups of interest, the action on $M$ fails to be free. There are two common methods for making an (effective) group action free. In geometry, this is accomplished by prolonging the action to a jet space $\mathrm{J}^n$ of suitably high order. The cross-section $\mathcal{K}$ is then an $r$-dimensional submanifold of $\mathrm{J}^n$, the normalization of the group parameters yields a standard moving frame $\rho^{(n)}\colon \mathrm{J}^n \to G$, and the invariantization of the jet coordinates $\iota(z^{(n)}) = I^{(n)}$ gives a complete set of differential invariants of order $\leq n$, [**27**]. The second possibility is to consider the product action of $G$ on a suitably large joint product $M^{\diamond k} \subset M^{\times k}$. The moving frame construction yields the *product frame* $\rho^{\diamond k}\colon M^{\diamond k} \to G$, and the invariantization of the coordinate functions $z_{N_i}$ gives a complete set of functionally independent joint invariants [**51**].

In [**50**], it is shown that the right geometrical space to study symmetry of numerical schemes is that of *multi-space*. The moving frame construction yields what is called a *multi-frame* and the invariantization map (3.5.2) gives *multi-invariants*. For the present discussion, it is enough to know that in the continuous limit $\rho^{\diamond k} \to \rho^{(n)}$ provided the moving frames are compatible. To obtain compatible moving frames, instead of working with the standard product action $Z_{N_l} = (X_{N_l}, U_{N_l}) = g \cdot z_{N_l}$ on $M^{\diamond k}$ we should consider the product action on the the finite difference coordinates

$$x_0^i,\, x_{N_1}^i, \ldots, x_{N_k}^i, \qquad u_0^\alpha, \qquad u^{d,(n)},$$

where $u^{d,(n)}$ denotes the collection of finite difference derivatives $u_J^{\alpha,d}$ of order $\leq n$ on an arbitrary mesh computed in Section 3.4. For the discrete invariants $(H_0, I^{d,(n)}) = \iota(x_0, u^{d,(n)})$ to converge to the differential invariants $(H, I^{(n)}) = \iota(x, u^{(n)})$, the cross-section $\mathcal{K}^{\diamond k}$ defining the product frame must, in the continuous limit, converge to a cross-section $\mathcal{K}^{(n)}$ for the prolonged action on $\mathrm{J}^n$. Assuming the action is transitive in the independent variables $x$, the limiting constraint on $\mathcal{K}^{\diamond k}$ implies that we can only normalize the independent variables at one multi-index, say $X_0 = c$, [**50**].

**Example 3.5.6.** To illustrate the above discussion we consider the symmetry group of the heat equation with logarithmic source: $u_t = u_{xx} + u \ln u$. The prolonged action induced by (3.3.8) is obtained by implementing the chain rule. The result is

$$(\ln U)_T = (\ln u)_t - \lambda_3 e^t x + \lambda_4 e^t - 2\lambda_3 e^t (\ln u)_x \qquad (\ln U)_X = (\ln u)_x - \lambda_3 e^t,$$
$$(\ln U)_{XX} = (\ln u)_{xx}, \tag{3.5.3}$$

and so on. Choosing the cross-section

$$\mathcal{K}^{(1)} = \{x = t = \ln u = (\ln u)_x = 0\}$$

and solving the normalization equations $X = T = \ln U = (\ln U)_X = 0$ for the group parameters $\lambda_1$, $\lambda_2$, $\lambda_3$, $\lambda_4$ yields the moving frame

$$\lambda_1 = -t, \qquad \lambda_2 = -(x + 2(\ln u)_x), \qquad \lambda_3 = e^{-t}(\ln u)_x,$$
$$\lambda_4 = e^{-t}(-\ln u + x(\ln u)_x + (\ln u)_x^2). \tag{3.5.4}$$

By construction

$$\iota(x) = \iota(t) = \iota(u) = \iota((\ln u)_x) = 0,$$

and the invariantization process yields the differential invariants

$$I = \iota((\ln u)_t) = \ln u_t - \ln u - (\ln u)_x^2, \qquad J = \iota((\ln u)_{xx}) = (\ln u)_{xx}, \tag{3.5.5}$$

and more.

We now repeat the computations for the discrete case. In the following, we assume that

$$t_{1,0} - t_{0,0} = 0 \tag{3.5.6}$$

as it simplifies the calculations. The equality (3.5.6) is compatible with the group action (3.3.8) as it is an invariant equation of the product action. To obtain a product frame compatible with (3.5.4) we choose the cross-section

$$\mathcal{K}^{\diamond 1} = \{x_{0,0} = t_{0,0} = u_{0,0} = (\ln u)_x^d = 0\}.$$

Working with centered difference derivatives in the $x$ variable,

$$(\ln u)^d_x = \frac{\ln u_{1,0} - \ln u_{-1,0}}{x_{1,0} - x_{-1,0}}$$

under assumption (3.5.6). Solving the corresponding normalization equations for the group parameters $\lambda_1$, $\lambda_2$, $\lambda_3$, $\lambda_4$ gives the product frame

$$\begin{gathered} \lambda_1 = -t_{0,0}, \qquad \lambda_2 = -(x_{0,0} + 2(\ln u)^d_x), \qquad \lambda_3 = e^{-t_{0,0}}(\ln u)^d_x, \\ \lambda_4 = e^{-t_{0,0}}\left[-\ln u_{0,0} + x_{0,0}(\ln u)^d_x + ((\ln u)^d_x)^2\right]. \end{gathered} \tag{3.5.7}$$

The invariantization map is then completely defined and yields, among many others, the discrete invariants

$$\begin{aligned} I^d &= \iota((\ln u)^d_t) = \frac{\ln u_{01} - e^\tau \ln u_{0,0}}{\tau} - \frac{\sigma}{\tau} e^\tau (\ln u)^d_x + \frac{e^\tau - e^{2\tau}}{\tau}((\ln u)^d_x)^2, \\ J^d &= \iota((\ln u)^d_{xx}) = (\ln u)^d_{xx}, \end{aligned} \tag{3.5.8}$$

where $\sigma = x_{0,1} - x_{0,0}$ and $\tau = t_{0,1} - t_{0,0}$, and

$$(\ln u)^d_{xx} = \frac{2}{x_{1,0} - x_{-1,0}}\left[\left(\frac{\ln u_{1,0} - \ln u_{0,0}}{x_{1,0} - x_{0,0}}\right) - \left(\frac{\ln u_{0,0} - \ln u_{-1,0}}{x_{0,0} - x_{-1,0}}\right)\right].$$

The discrete invariant

$$\iota(x_{0,1}) = \sigma + 2(e^\tau - 1)(\ln u)^d_x \tag{3.5.9}$$

will also prove to be useful in the construction of an invariant numerical scheme in the following section.

## 3.6. Invariant Numerical Schemes

Let $\Delta_\nu(x, u^{(n)}) = 0$ be a $G$-invariant system of differential equations as defined in Definition 3.3.3. The invariance of the system guarantees that it can be expressed in terms of the normalized invariants $\iota(x, u^{(n)}) = (H, I^{(n)})$. Using the invariantization map (3.5.2)

$$0 = \Delta_\nu(x, u^{(n)}) = \iota(\Delta_\nu(x, u^{(n)})) = \Delta_\nu(H, I^{(n)}). \tag{3.6.1}$$

To obtain an invariant numerical scheme we simply need to replace the differential invariants $(H, I^{(n)})$ in (3.6.1) by their invariant discrete counterparts $\iota(x_0, u^{d,(n)}) = (H_0, I^{d,(n)})$ and add equations specifying the mesh. If the equations determining the mesh are invariant under the group action $G$, the scheme is said to be *fully invariant*, otherwise it is called *partially invariant*. In applications, invariant constraints on the mesh are usually specified with the aim of simplifying the expressions of the invariant scheme. This is illustrated in Examples 3.6.1 and 3.6.2.

An alternative way of constructing the same invariant numerical scheme consists of replacing the partial derivatives in the differential equations $\Delta_\nu(x, u^{(n)}) = 0$ by their finite difference approximation

$$\Delta_\nu(x, u^{(n)}) = 0 \qquad \longrightarrow \qquad E_\nu = \Delta_\nu(x_{0,0}, u^{d,(n)}) = 0, \tag{3.6.2}$$

followed by the invariantization of (3.6.2).

**Example 3.6.1.** The heat equation (3.3.2) with logarithmic source is easily expressed in terms of the differential invariants (3.5.5). By invariantizing (3.3.2), the equation can be rewritten as

$$0 = \iota(u_t - u_{xx} - u \ln u) = I - J. \tag{3.6.3}$$

To obtain an invariant discrete version, $I$ and $J$ in (3.6.3) are simply replaced by their discrete counterparts:

$$I^d - J^d = \frac{\ln u_{0,1} - e^\tau \ln u_{0,0}}{\tau} - \frac{\sigma}{\tau} e^\tau (\ln u)^d_x + \frac{e^\tau - e^{2\tau}}{\tau}((\ln u)^d_x)^2 - (\ln u)^d_{xx} = 0. \tag{3.6.4}$$

By construction, the numerical scheme is a valid approximation of (3.3.2) on any mesh satisfying the flat time assumption (3.5.6). At the moment, there is no systematic method for obtaining invariant equations defining the mesh of an invariant numerical scheme. In **[32]** it is claimed that the equations for the invariant mesh are obtained by invariantizing the mesh equations for the corresponding non-invariant numerical scheme. The issue with this proposition is that there is no guarantee that the equations obtained after invariantization are compatible. Indeed, this idea was used in [**14**] and led to the incompatible mesh equations (83–85). To illustrate the problem we invariantize the equations (3.3.4b) describing a uniform rectangular mesh. The result is

$$x_{1,0} - x_{0,0} = h, \qquad x_{0,1} - x_{0,0} = \sigma = 2(\ln u)^d_x(1 - e^\tau),$$

$$t_{1,0} - t_{0,0} = 0, \qquad t_{0,1} - t_{0,0} = \tau = k.$$

In the time variable $t$ the mesh equations are compatible but this is not the case in the spatial variable $x$. By shifting the first equation by $\delta$ and the second equation by $\Delta$ (recall (3.4.5)) we obtain the constraint

$$h = x_{1,1} - x_{0,1} = 2\Delta[(\ln u)_x](1 - e^k). \tag{3.6.5}$$

Since $h$ and $k$ are constants, equation (3.6.5) imposes a restriction on the solution $u$ which is not admissible. To circumvent the problem we can neglect equation $x_{10} - x_{0,0} = h$ and assume that the mesh equations are given by

$$\sigma = 2(1 - e^\tau)(\ln u)^d_x, \qquad \tau = k, \qquad \Delta t = 0. \tag{3.6.6}$$

With (3.6.6), the mesh is uniquely determined once the sample points in $x$ are fixed at some time $t = t_0$. In conclusion, a fully invariant numerical numerical scheme for the heat equation (3.3.2) is given by

$$\begin{gathered} E_1 = \frac{\ln u_{0,1} - e^\tau \ln u_{0,0}}{\tau} - e^\tau \frac{1 - e^\tau}{\tau}((\ln u)^d_x)^2 - (\ln u)^d_{xx} = 0, \\ E_2 = \sigma - 2(1 - e^\tau)(\ln u)^d_x = 0, \qquad E_3 = \tau - k = 0, \qquad E_4 = \Delta t = 0. \end{gathered} \tag{3.6.7}$$

**Example 3.6.2.** In this example we construct an invariant numerical scheme for the spherical Burgers' equation

$$u_t + \frac{u}{t} + uu_x + u_{xx} = 0, \qquad t > 0. \tag{3.6.8}$$

The differential equation (3.6.8) admits the three-dimensional Lie algebra of infinitesimal symmetry generators, [**1**],

$$\mathbf{v}_1 = \frac{\partial}{\partial x}, \qquad \mathbf{v}_2 = x\frac{\partial}{\partial x} + 2t\frac{\partial}{\partial t} - u\frac{\partial}{\partial u}, \qquad \mathbf{v}_3 = \ln t\frac{\partial}{\partial x} + \frac{1}{t}\frac{\partial}{\partial u}.$$

The corresponding group action is

$$X = e^{\lambda_2}(x + \lambda_3 \ln t) + \lambda_1, \qquad T = e^{2\lambda_2}t, \qquad U = e^{-\lambda_2}\left(u + \frac{\lambda_3}{t}\right). \tag{3.6.9}$$

For the joint action, a simple choice of cross-section is

$$x_{0,0} = 0, \qquad t_{0,0} = 1, \qquad u_{0,0} = 0.$$

Solving the normalization equations

$$X_{0,0} = 0, \qquad T_{0,0} = 1, \qquad U_{0,0} = 0$$

for the group parameters yields the product frame

$$\lambda_1 = -\frac{x_{0,0} - u_{0,0}t_{0,0}\ln t_{0,0}}{\sqrt{t_{0,0}}}, \qquad \lambda_2 = \ln\left(\frac{1}{\sqrt{t_{0,0}}}\right), \qquad \lambda_3 = -u_{0,0}t_{0,0}. \tag{3.6.10}$$

An invariant numerical scheme for the spherical Burgers' equation (3.6.8) is obtain by invariantizing the discrete derivatives $u^d_{xx}$ and $u^d_t$:

$$0 = I^d = \iota(u^d_t) + \iota(u^d_{xx}) = u^d_t + \frac{u_{0,0}}{t_{0,0}} + u_{0,0}u^d_x + u^d_{xx}. \tag{3.6.11}$$

The equation (3.6.11) is defined on any compatible mesh. We now impose some invariant constraints on the mesh which will simplify the coordinate expressions of (3.6.11). Once more, we assume that $\Delta t_{0,0} = t_{1,0} - t_{0,0} = 0$ as this constraint is invariant under the group action (3.6.9). Another invariant constraint is given by $\delta^2 t_{0,0} = t_{0,2} - 2t_{0,1} + t_{0,0} = 0$. Finally, using the invariant

$$\iota(x_{0,1}) = x_{0,1} - x_{0,0} - ut\ln\left(\frac{t_{0,1}}{t_{0,0}}\right) = \sigma - u_{0,0}t_{0,0}\ln\left(\frac{t_{0,1}}{t_{0,0}}\right),$$

an invariant mesh is specified by the equations

$$\sigma = u_{0,0}t_{0,0}\ln\left(\frac{t_{0,1}}{t_{0,0}}\right), \qquad \Delta t_{0,0} = 0, \qquad \delta^2 t_{0,0} = 0. \tag{3.6.12}$$

As in the previous example, once the sample points in $x$ are determined at some time $t = t_0$ and the constant step size $\tau = k$ in $t$ is chosen, the equations (3.6.12) uniquely fix the mesh. On the mesh (3.6.12), equation (3.6.11) simplifies to the fully invariant numerical scheme

$$\begin{gathered} E_1 = u_{0,1} - \frac{u_{0,0}t_{0,0}}{t_{0,1}} + 2\tau u^d_{xx} = 0, \\ E_2 = \sigma - u_{0,0}t_{0,0}\ln\left(\frac{t_{0,1}}{t_{0,0}}\right) = 0, \qquad E_3 = \Delta t_{0,0} = 0, \qquad E_4 = \delta^2 t_{0,0} = 0, \end{gathered} \tag{3.6.13}$$

where

$$u^d_{xx} = \frac{2}{x_{1,0} - x_{-1,0}}\left[\left(\frac{u_{1,0} - u_{0,0}}{x_{1,0} - x_{0,0}}\right) - \left(\frac{u_{0,0} - u_{-1,0}}{x_{0,0} - x_{-1,0}}\right)\right].$$

## 3.7. Numerical Tests

Fully invariant numerical schemes for the heat equation with logarithmic source (3.3.2) and the spherical Burgers' equation (3.6.8) were obtained in (3.6.7) and (3.6.13), respectively. To illustrate how preservation of symmetry can increase the accuracy of a numerical method, we compare the fully invariant schemes with two closely related schemes. Firstly, recall that provided the flat time assumption (3.5.6) holds, the discretizations (3.6.4) and (3.6.11) are valid approximations of the corresponding partial differential equation on any compatible mesh. To gauge the effect of imposing invariant constraints on the mesh, we compare the fully invariant schemes to partially invariant schemes obtained by restricting (3.6.4) and (3.6.11) to non-invariant uniform rectangular meshes. Then, for further comparison, the fully and partially invariant schemes are set against standard finite difference approximations on uniform rectangular meshes.

### 3.7.1. Heat Equation

For the heat equation (3.3.2) we used the time-independent solution

$$u(x,t) = \exp\left[-\frac{x^2}{4} + \frac{1}{2}\right] \tag{3.7.1}$$

to compare the precision of the three schemes. Starting at $t = 0$ and working on the space interval $[-5, 5]$, the solution after one unit of time elapsed is shown in Figure 3.3. The numerical simulation was done using an initial spacial step size of $h = 0.15$ and a constant time step $\tau = k = 0.001$. We note that for the fully invariant scheme (3.6.7) the mesh evolves according to the equation

$$\sigma = 2(1 - e^{\tau})(\ln u)_x^d.$$

The result is an expansion of the space interval $[-5, 5]$ over the course of the simulation as shown in Figure 3.4. The absolute errors for the three numerical schemes are given in Figure 3.5. As anticipated, the standard numerical scheme offers the worst precision among the three. The accuracy of the partially invariant scheme on a rectangular mesh is comparable to the fully invariant numerical scheme, but the latter gives slightly better results.

### 3.7.2. Burgers' Equation

For the spherical Burgers' equation (3.6.8), a numerical test was performed using the solution

$$u(x,t) = \frac{x + c_1}{t(c_2 + \ln t)} \qquad \text{with} \qquad c_1 = 0 \quad \text{and} \quad c_2 = 1.$$

At $t = 1$, the initial step sizes chosen are $h = 0.5$ in $x$ and $\tau = k = 0.001$ in $t$. In Figure 3.6, the solution is shown at $t = 1.5$. As in the previous simulation, the mesh of the fully invariant numerical scheme evolves as a function of time (see Figure 3.7).

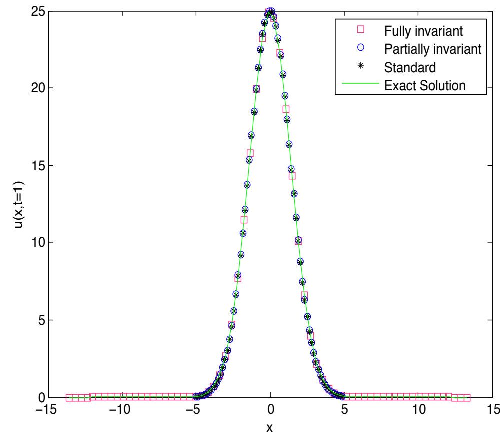



FIG. 3.3. Solution $u = \exp[x^2/4 + 1/2]$.

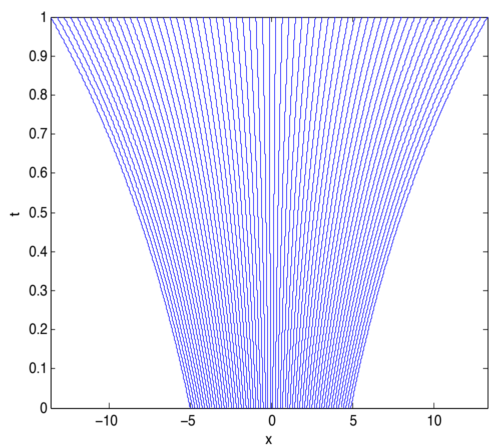



FIG. 3.4. Invariant mesh.

The evolution is governed by the equation

$$\sigma = u_{0,0} t_{0,0} \ln\left(\frac{t_{0,1}}{t_{0,0}}\right).$$

The absolute errors for the three numerical schemes are given in Figures 3.8 and 3.9. Once more, the fully invariant scheme is more precise. For the solution considered the improvement is considerable as the error is reduced by a factor $10^{-13}$

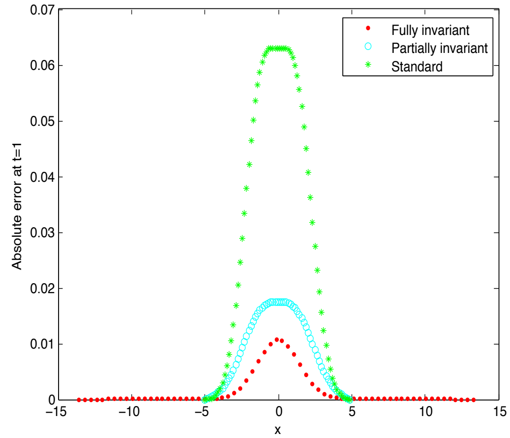



FIG. 3.5. Absolute errors for the solution $u = \exp[x^2/4 + 1/2]$.

compared with the two other schemes. On the other hand, while the partially invariant scheme is slightly more accurate than the standard scheme, the errors are comparable.

## 3.8. Concluding Remarks

Other simulations, not included in the paper, indicate that invariant schemes do not always improve the numerical accuracy when compared to standard schemes. While the error is generally not worst than the standard scheme it is still not clear for which types of equations or solutions an invariant scheme will give significantly better results. Knowing when this is the case would be useful for future applications.

As with all other works on the subject, the important question of the stability of an invariant scheme was not addressed in this paper. At the moment it is not clear how the evolution of the mesh affects the stability.

Finally, many partial differential equations admit infinite-dimensional symmetry groups. Classical examples include the Kadomtsev–Petviashvili equation [**15**], the Infeld–Rowlands equation [**25**] and the Davey–Stewartson equations [**12**]. It would

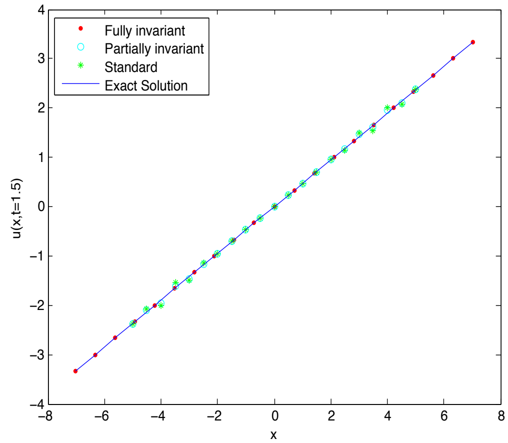



FIG. 3.6. Solution $u = x/[t(1+\ln t)]$.

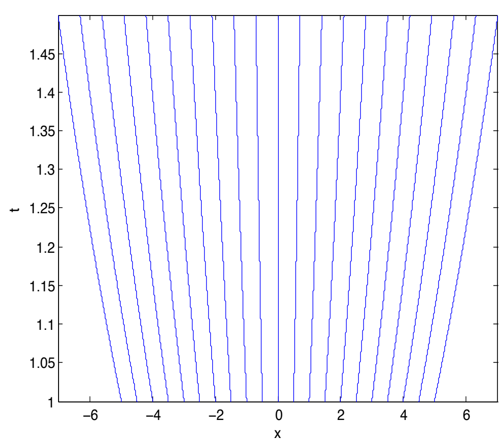



FIG. 3.7. Invariant mesh.

be of great interest to find a procedure for constructing invariant numerical schemes of partial differential equations admitting an infinite-dimensional symmetry group.

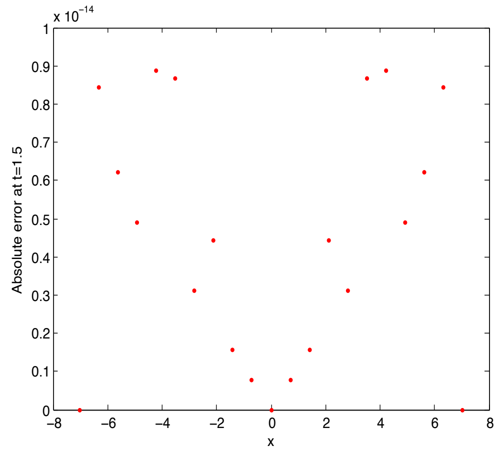



FIG. 3.8. Absolute error for the fully invariant scheme.

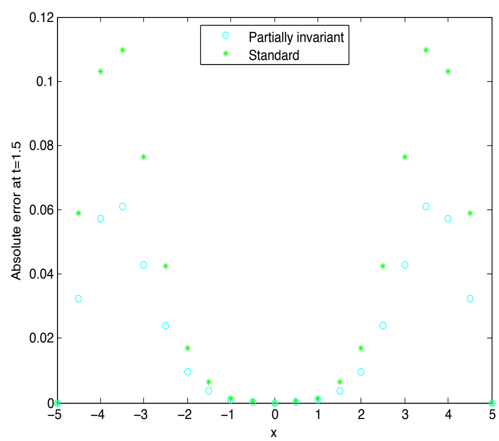



FIG. 3.9. Absolute errors for the standard and partially invariant schemes.

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# Chapter 4

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## Invariant Discretization of Partial Differential Equations Admitting Infinite-Dimensional Symmetry Groups

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## 4.1. Abstract

This paper is concerned with the invariant discretization of differential equations admitting infinite-dimensional symmetry groups. By way of example, we first show that there are differential equations with infinite-dimensional symmetry groups that do not admit enough joint invariants preventing the construction of invariant finite difference approximations. To solve this shortage of joint invariants we propose to discretize the pseudo-group action. Computer simulations indicate that the numerical schemes constructed from the joint invariants of discretized pseudo-group can produce better numerical results than standard schemes.

## 4.2. Introduction

For the last 20 years, a considerable amount of work has been invested into the problem of invariantly discretizing differential equations with symmetries. This effort is part of a larger program aiming to extend Lie's theory of transformation groups to finite difference equations, [**40**]. With the emergence of physical models based on discrete spacetime, and in light of the importance of symmetry in our understanding of modern physics, the problem of invariantly discretizing differential equations is still of present interest. From a theoretical standpoint, working with invariant numerical schemes allows one to use standard Lie group techniques to find explicit solutions, [**65**], or compute conservation laws, [**21**]. From a more practical point of view, the motivation stems from the fact that invariant schemes have been shown to outperform standard numerical methods in a number of examples, [**8, 16, 33, 63**].

In general, to build an invariant numerical scheme one has to construct joint invariants (also known as finite difference invariants). These joint invariants are usually found using one of two methods. One can either use Lie's method of infinitesimal generators which requires solving a system of linear partial differential equations, [**22, 40**], or the method of equivariant moving frames which requires solving a system of (nonlinear) algebraic equations, [**33, 50**]. Both approaches produce joint invariants which, in the coalescent limit, converge to differential invariants of the prolonged action. Thus far, the theory and applications found in the literature primarily deal with finite-dimensional Lie group actions and the case of infinite-dimensional Lie pseudo-groups as yet to be satisfactorily treated. Many partial differential equations in hydrodynamics or meteorology admit infinite-dimensional symmetry groups. The Navier–Stokes equation, [**48**], the Kadomtsev–Petviashvili equation, [**15**], and the Davey–Stewartson equations, [**12**], are classical examples of such equations. Linear or linearizable partial differential equations also form a large class of equations admitting infinite-dimensional symmetry groups.

To construct invariant numerical schemes of differential equations admitting symmetries, one of the main steps consists of finding joint invariants that approximate the differential invariants of the symmetry group. For finite-dimensional Lie group actions, this can always be done by considering the product action on sufficiently many points. Unfortunately, as the next example shows, the same is not true for infinite-dimensional Lie pseudo-group actions.

**Example 4.2.1.** Let $f(x) \in \mathcal{D}(\mathbb{R})$ be a local diffeormorphism of $\mathbb{R}$. Throughout the paper we will use the infinite-dimensional pseudo-group

$$X = f(x), \qquad Y = y, \qquad U = \frac{u}{f'(x)}, \tag{4.2.1}$$

acting on $\mathbb{R}^3 \setminus \{u = 0\}$, to illustrate the theory and constructions. The pseudo-group (4.2.1) was introduced by Lie, [**43**, p.373], in his study of second order partial differential equations integrable by the method of Darboux. It also appears in Vessiot's work on group splitting and automorphic systems, [**68**], in Kumpera's investigation of Lie's theory of differential invariants based on Spencer's cohomology, [**34**], and recently in [**52, 54, 59**] to illustrate a new theoretical foundation of moving frames.

The differential invariants of the pseudo-group action (4.2.1) can be found in [**54**]. One of these invariants is

$$I_{1,1} = \frac{u\,u_{xy} - u_x\,u_y}{u^3}. \tag{4.2.2}$$

With (4.2.2) it is possible to form the partial differential equation

$$\frac{u\,u_{xy} - u_x\,u_y}{u^3} = 1, \tag{4.2.3}$$

which was used in [**59**] to illustrate the method of symmetry reduction of exterior differential systems.

By construction, Equation (4.2.3) is invariant under the pseudo-group[1] (4.2.1). To obtain an invariant discretization of (4.2.3), an invariant approximation of the differential invariant (4.2.2) must be found. To discretize the invariant (4.2.2), the multi-index $(m,n) \in \mathbb{Z}^2$ is introduced to label sample points:

$$x_{m,n}, \qquad y_{m,n}, \qquad u_{m,n} = u(x_{m,n}, y_{m,n}). \tag{4.2.4}$$

Following the general philosophy, [**22, 33, 40, 50**], the pseudo-group (4.2.1) induces the product action

$$X_{m,n} = f(x_{m,n}), \qquad Y_{m,n} = y_{m,n}, \qquad U_{m,n} = \frac{u_{m,n}}{f'(x_{m,n})} \tag{4.2.5}$$

on the discrete points (4.2.4). On an arbitrary finite set of points, we claim that the only joint invariants are

$$Y_{m,n} = y_{m,n}. \tag{4.2.6}$$

To see this, let $\mathcal{N}$ be a finite subset of $\mathbb{Z}^2$, and assume $x_{m,n} \in \operatorname{dom} f$ for $(m,n) \in \mathcal{N}$. Since the components $x_{m,n}$ are generically distinct and $f \in \mathcal{D}(\mathbb{R})$ is an arbitrary local diffeomorphism, the *pseudo-group parameters*

$$f(x_{m,n}) \quad \text{and} \quad f'(x_{m,n}) \quad \text{with} \quad (m,n) \in \mathcal{N} \tag{4.2.7}$$

[1]Equation (4.2.3) admits a larger symmetry group given by $X = f(x)$, $Y = g(y)$, $U = u/(f'(x)\,g'(y))$, with $f,\, g \in \mathcal{D}(\mathbb{R})$. This pseudo-group is considered in Example 4.4.20.

are independent. Hence, as shown in [**30**], the pseudo-group (4.2.5) shares the same invariants as its Lie completion

$$X_{m,n} = f_{m,n}(x_{m,n}), \qquad Y_{m,n} = y_{m,n}, \qquad U_{m,n} = \frac{u_{m,n}}{f'_{m,n}(x_{m,n})}, \tag{4.2.8}$$

where for each different subscript $(m,n) \in \mathcal{N}$, the functions $f_{m,n} \in \mathcal{D}(\mathbb{R})$ are functionally independent local diffeomorphisms[2]. For the Lie completion (4.2.8), it is clear that (4.2.6) are the only admissible invariants. Hence, generically, we conclude that it is not possible to approximate the differential invariant (4.2.2) by joint invariants.

To construct additional joint invariants, invariant constraints on the independent variables $x_{m,n}$ need to be imposed to reduce the number of pseudo-group parameters (4.2.7). To reduce this number as much as possible, we assume that

$$x_{m,n+1} = x_{m,n}. \tag{4.2.9}$$

Equation (4.2.9) is seen to be invariant under the product action (4.2.5) since

$$X_{m,n+1} = f(x_{m,n+1}) = f(x_{m,n}) = X_{m,n}$$

when (4.2.9) holds. Equation (4.2.9) implies that $x_{m,n}$ is independent of the index $n$:

$$x_{m,n} = x_m.$$

To cover (a region of) the $xy$-plane,

$$\Delta x_m = x_{m+1} - x_m \neq 0 \qquad \text{and} \qquad \delta y_{m,n} = y_{m,n+1} - y_{m,n} \neq 0$$

[2]It is customary to use the notation $f_{m,n} = f(x_{m,n})$ to denote the value of the function $f(x)$ at the point $x_{m,n}$, and this is the convention used in Sections 4.4, 4.5, and 4.6. In equation (4.2.8), the subscript attached to the diffeomorphism $f_{m,n}(x_{m,n})$ has a different meaning. Here, the subscript $(m,n)$ is used to denote different diffeomorphisms. Thus, the pseudo-group (4.2.5) is contained in the Lie completion (4.2.8). This particular use of the subscript only occurs in (4.2.8).

must hold. Since the variables $y_{m,n}$ are invariant under the product action (4.2.5) we can, for simplicity, set

$$y_{m,n} = y_n = k\,n + y_0, \tag{4.2.10}$$

where $k > 0$ and $y_0$ are constants. To respect the product action (4.2.5) we cannot require the step size $\Delta x_m = x_{m+1} - x_m$ to be constant as this is not an invariant assumption of the pseudo-group action. Thus, in general, the mesh in the independent variables $(x_m, y_n)$ will be rectangular with variable step sizes in $x$, see Figure 4.1.

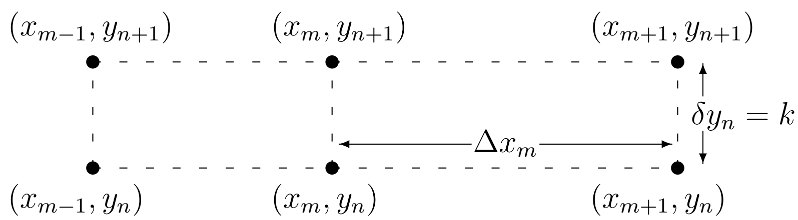



FIG. 4.1. Rectangular mesh.

Repeating the argument above, when (4.2.9) and (4.2.10) hold, the joint invariants of the product action (4.2.5) are

$$y_n, \qquad \frac{u_{m,n+k}}{u_{m,n}}, \qquad k,\, m,\, n \in \mathbb{Z}. \tag{4.2.11}$$

Introducing the dilation group

$$X = x, \qquad Y = y, \qquad U = \lambda\, u, \qquad \lambda > 0, \tag{4.2.12}$$

we see that the differential invariant (4.2.2) cannot be approximated by the joint invariants (4.2.11). Indeed, since the invariants $u_{m,n+k}/u_{m,n}$ are homogeneous of degree 0, any combination of the invariants (4.2.11) will converge to a differential invariant of homogeneous degree 0. On the other hand, the differential invariant (4.2.2) is homogeneous of degree $-1$ under (4.2.12).

As it stands, it is not possible to construct joint invariants that approximate the differential invariant (4.2.2). To remedy the problem, one possibility is to reduce the size of the symmetry group by considering sub-pseudo-groups. For the diffeomorphism pseudo-group $\mathcal{D}(\mathbb{R})$, since the largest non-trivial sub-pseudo-group is the special linear group $SL(2)$, [**49**], this approach drastically changes the nature of the action as it transitions from an infinite-dimensional transformation group to a three-dimensional group of transformations. In this paper we are interested in preserving the infinite-dimensional nature of transformation groups and propound another suggestion. Taking the point of view that the notion of derivative is not defined in the discrete setting, we propose to discretize infinite-dimensional pseudo-group actions. In other words, derivatives are to be replaced by finite difference approximations. For the pseudo-group (4.2.1), instead of considering the product action (4.2.5), we suggest to work with the first order approximation

$$X_m = f(x_m), \qquad Y_n = y_n = k\,n + y_0, \qquad U_{m,n} = u_{m,n} \cdot \frac{x_{m+1} - x_m}{f(x_{m+1}) - f(x_m)}. \tag{4.2.13}$$

In Section 4.4, joint invariants of the pseudo-group action (4.2.13) are constructed and an invariant numerical scheme approximating (4.2.3) is obtained in Section 4.5.

To develop our ideas we opted to use the theory of equivariant moving frames, [**50, 54**], but our constructions can also be recast within Lie's infinitesimal framework. In Section 4.3, the concept of an infinite-dimensional Lie pseudo-group is recalled and the equivariant moving frame construction is summarized. In Section 4.4, pseudo-group actions are discretized and the equivariant moving frame construction is adapted to those actions. Along with (4.2.1), the pseudo-group

$$X = f(x), \qquad Y = y\,f'(x) + g(x), \qquad U = u + \frac{y\,f''(x) + g'(x)}{f'(x)}, \tag{4.2.14}$$

with $f \in \mathcal{D}(\mathbb{R})$ and $g \in C^\infty(\mathbb{R})$, will stand as a second example to illustrate our constructions. We choose to work with the pseudo-groups (4.2.1) and (4.2.14) to keep our examples relatively simple. Furthermore, these pseudo-groups have been extensively used in [**52, 54, 55, 56**] to illustrate the (continuous) method of moving frames. With these well-documented examples, it allowed us to verify that our discrete constructions and computations did converge to their continuous counterparts.

Finally, in Section 4.6 an invariant numerical approximation of (4.2.3) is compared to a standard discretization of the equation. Our numerical tests show that the invariant scheme is more precise and stable than the standard scheme.

## 4.3. Lie Pseudo-groups and moving frames

For completeness, we begin by recalling the definition of a pseudo-group, [**11, 34, 35, 52, 54, 66**]. Let $M$ be an $m$-dimensional manifold. By a local diffeomorphism of $M$ we mean a one-to-one map $\varphi\colon U \to V$ defined on open subsets $U$, $V = \varphi(U) \subset M$, with inverse $\varphi^{-1}\colon V \to U$.

**Definition 4.3.1.** A collection $\mathcal{G}$ of local diffeomorphisms of $M$ is a *pseudo-group* if

- $\mathcal{G}$ is closed under restriction: if $U \subset M$ is an open set and $g\colon U \to M$ is in $\mathcal{G}$, then so is the restriction $g|_V$ for all open $V \subset U$.
- Elements of $\mathcal{G}$ can be pieced together: if $U_\nu \subset M$ are open subsets, $U = \bigcup_\nu U_\nu$, and $g\colon U \to M$ is a local diffeomorphism with $g|_{U_\nu} \in \mathcal{G}$ for all $\nu$, then $g \in \mathcal{G}$.
- $\mathcal{G}$ contains the identity diffeomorphism: $\mathbb{1} \cdot z = z$ for all $z \in M = \operatorname{dom} \mathbb{1}$.
- $\mathcal{G}$ is closed under composition: if $g\colon U \to M$ and $h\colon V \to M$ are two diffeomorphisms belonging to $\mathcal{G}$, and $g(U) \subset V$, then $h \cdot g \in \mathcal{G}$.
- $\mathcal{G}$ is closed under inversion: if $g\colon U \to M$ is in $\mathcal{G}$ then so is $g^{-1}\colon g(U) \to M$.

**Example 4.3.2.** One of the simplest pseudo-group is given by the collection of local diffeomorphisms $\mathcal{D} = \mathcal{D}(M)$ of a manifold $M$. All other pseudo-groups defined on $M$ are sub-pseudo-groups of $\mathcal{D}$.

For $0 \leq n \leq \infty$, let $\mathcal{D}^{(n)} = \mathrm{J}^{(n)}(M, M)$ denote the bundle formed by the $n^{\text{th}}$ order jets of local diffeomorphisms of $M$. Local coordinates on $\mathcal{D}^{(n)}$ are given by $\varphi^{(n)}|_z = (z, Z^{(n)})$, where $z = (z^1, \ldots, z^m)$ are the source coordinates of the local diffeomorphism, $Z = \varphi(z)$, $Z = (Z^1, \ldots, Z^m)$ its target coordinates, and $Z^{(n)}$ collects the derivatives of the target coordinates $Z^a$ with respect to the source coordinates $z^b$ of order $\leq n$. For $k \geq n$, the standard projection is denoted $\widetilde{\pi}^k_n \colon \mathcal{D}^{(k)} \to \mathcal{D}^{(n)}$.

**Definition 4.3.3.** A pseudo-group $\mathcal{G} \subset \mathcal{D}$ is called a *Lie pseudo-group* of order $n^\star \geq 1$ if, for all finite $n \geq n^\star$:

- $\mathcal{G}^{(n)} \subset \mathcal{D}^{(n)}$ forms a smooth embedded subbundle,
- the projection $\widetilde{\pi}^{n+1}_n \colon \mathcal{G}^{(n+1)} \to \mathcal{G}^{(n)}$ is a fibration,
- every local diffeomorphism $g \in \mathcal{D}$ satisfying $g^{(n^\star)} \subset \mathcal{G}^{(n^\star)}$ belongs to $\mathcal{G}$,
- $\mathcal{G}^{(n)} = \mathrm{pr}^{(n-n^\star)}\mathcal{G}^{(n^\star)}$ is obtained by prolongation.

In local coordinates, the subbundle $\mathcal{G}^{(n^\star)} \subset \mathcal{D}^{(n^\star)}$ is characterized by a system of $n^{\star\,\text{th}}$ order (formally integrable) partial differential equations

$$F^{(n^\star)}(z, Z^{(n^\star)}) = 0, \tag{4.3.1}$$

called the $n^{\star\,\text{th}}$ order *determining system* of the pseudo-group. A Lie pseudo-group is said to be of *finite type* if the solution space of (4.3.1) only involves a finite number of arbitrary constants. Lie pseudo-groups of finite type are thus isomorphic to local Lie group actions. On the other hand, a Lie pseudo-group is of *infinite type* if it involves arbitrary functions.

**Remark 4.3.4.** Linearizing (4.3.1) at the identity jet $\mathbb{1}^{(n^\star)}$ yields the *infinitesimal determining equations*

$$L^{(n^\star)}(z, \zeta^{(n^\star)}) = 0 \tag{4.3.2}$$

for an infinitesimal generator

$$\mathbf{v} = \sum_{a=1}^{m} \zeta^a(z) \frac{\partial}{\partial z^a}. \tag{4.3.3}$$

The vector field (4.3.3) is in the Lie algebra $\mathfrak{g}$ of infinitesimal generators of $\mathcal{G}$ if its components are solution of (4.3.2). Given a differential equation $\Delta(x, u^{(n)}) = 0$ with symmetry group $\mathcal{G}$, the infinitesimal determining system (4.3.2) is equivalent to the equations obtained by Lie's standard algorithm for determining the symmetry algebra of the differential equation $\Delta = 0$, [**48**].

**Example 4.3.5.** The pseudo-group (4.2.1) is a Lie pseudo-group. The first order determining equations are

$$\begin{gathered} X_y = X_u = 0, \qquad Y = y, \qquad Y_x = Y_u = 0, \qquad Y_y = 1, \\ U X_x = u, \qquad U_u X_x = 1, \qquad U_y = 0. \end{gathered} \tag{4.3.4}$$

If

$$\mathbf{v} = \xi(x,y,u)\frac{\partial}{\partial x} + \eta(x,y,u)\frac{\partial}{\partial y} + \varphi(x,y,u)\frac{\partial}{\partial u}$$

denotes a (local) vector fields in $\mathbb{R}^3 \setminus \{u = 0\}$, the linearization of (4.3.4) at the identity jet yields the first order infinitesimal determining equations

$$\xi_y = \xi_u = 0, \quad \eta = \eta_x = \eta_y = \eta_u = 0, \quad \varphi = -u\,\xi_x, \quad \varphi_y = 0, \quad \varphi_u = -\xi_x.$$

The general solution to this system of equations is

$$\mathbf{v} = a(x)\frac{\partial}{\partial x} - u\,a'(x)\frac{\partial}{\partial u},$$

where $a(x)$ is an arbitrary smooth function.

Given a Lie pseudo-group $\mathcal{G}$ acting on $M$, we are now interested in the induced action on $p$-dimensional submanifolds $S \subset M$ with $1 \leq p < m = \dim M$. It is customary to introduce adapted coordinates

$$z = (x, u) = (x^1, \ldots, x^p, u^1, \ldots, u^q) \tag{4.3.5}$$

on $M$ so that, locally, a submanifold $S$ transverse to the vertical fibre $\{x = x_0\}$ is given as the graph of a function $S = \{(x, u(x))\}$. For each integer $0 \leq n \leq \infty$, let $\mathrm{J}^{(n)} = \mathrm{J}^{(n)}(M, p)$ denote the $n^{\text{th}}$ order *submanifold jet bundle* defined as the set of equivalence classes under the equivalence relation of $n^{\text{th}}$ order contact, [**49**]. For $k \geq n$, let $\pi^k_n \colon \mathrm{J}^{(k)} \to \mathrm{J}^{(n)}$ denote the canonical projection. In the adapted system of coordinates $z = (x, u)$, coordinates on $\mathrm{J}^{(n)}$ are given by

$$z^{(n)} = (x, u^{(n)}) = (\ldots\ x^i\ \ldots\ u^\alpha_{x^J}\ \ldots), \tag{4.3.6}$$

where $u^{(n)}$ denotes the collection of derivatives $u^\alpha_{x^J}$ of order $0 \leq \#J \leq n$.

Alternatively, when no distinction between dependent and independent variables is made, a submanifold $S \subset M$ can be locally parameterized by $p$ variables $s = (s^1, \ldots, s^p) \in \mathbb{R}^p$ so that

$$z(s) = (x(s), u(s)) \in S.$$

In the numerical analysis community, the variables $s = (s^1, \ldots, s^p)$ are called *computational variables*, [**28**]. We let $\mathcal{J}^{(n)}$ denote the $n^{\text{th}}$ order jet space of submanifolds $S \subset M$ parametrized by computational variables. Local coordinates on $\mathcal{J}^{(n)}$ are given by

$$\mathfrak{z}^{(n)} = (s, x^{(n)}, u^{(n)}) = (\ldots\ s^i\ \ldots\ x^i_{s^A}\ \ldots\ u^\alpha_{s^A}\ \ldots), \tag{4.3.7}$$

with $1 \leq i \leq p$, $1 \leq \alpha \leq q$, and $0 \leq \#A \leq n$. The transition between the jet coordinates (4.3.6) and (4.3.7) is given by the chain rule. Provided

$$\det\left(\frac{\partial x^i}{\partial s^j}\right) \neq 0, \tag{4.3.8}$$

successive application of the implicit total differential operators

$$D_{x^i} = \sum_{j=1}^{p} W_i^j \, D_{s^j}, \qquad \big(W_i^j\big) = \big(x^j_{s^i}\big)^{-1}, \tag{4.3.9}$$

to the dependent variables $u^\alpha$ will give the coordinate expressions for the $x$ derivatives of $u$ in terms of the $s$ derivatives of $x$ and $u$:

$$u^\alpha_{x^J} = D_{x^{j_1}} \cdots D_{x^{j_k}} u^\alpha = \left( \sum_{\ell=1}^{p} W^\ell_{j_1} \, D_{s^\ell} \right) \cdots \left( \sum_{\ell=1}^{p} W^\ell_{j_k} \, D_{s^\ell} \right) u^\alpha. \tag{4.3.10}$$

Given a Lie pseudo-group $\mathcal{G}$ acting on $M$, the action is prolonged to the computational variables by requiring that they remain unchanged:

$$g \cdot (s, z) = (s, g \cdot z) \qquad \text{for all} \qquad g \in \mathcal{G}.$$

By abuse of notation we still use $\mathcal{G}$ to denote the extended action $\{\mathbb{1}\} \times \mathcal{G}$ on $\mathbb{R}^p \times M$.

The complete theory of moving frames for infinite-dimensional Lie pseudo-groups can be found in [**54**]. For reasons that will become more apparent in the next section we recall the main constructions over the jet bundle $\mathcal{J}^{(n)}$ rather than $\mathrm{J}^{(n)}$. Using (4.3.10) one can translate the constructions from $\mathcal{J}^{(n)}$ to $\mathrm{J}^{(n)}$. Let

$$\mathcal{B}^{(n)} = \mathcal{J}^{(n)} \times_M \mathcal{G}^{(n)} \tag{4.3.11}$$

denote the $n^{\text{th}}$ order *lifted bundle*. Local coordinates on $\mathcal{B}^{(n)}$ are given by $(\mathfrak{z}^{(n)}, g^{(n)})$, where the base coordinates are the submanifold jet coordinates $\mathfrak{z}^{(n)} = (s, x^{(n)}, u^{(n)}) \in \mathcal{J}^{(n)}$ and the fibre coordinates are the pseudo-group parameters $g^{(n)}$ where $(x, u) \in \operatorname{dom} g$. A local diffeomorphism $h \in \mathcal{G}$ acts on $\mathcal{B}^{(n)}$ by right multiplication:

$$R_h(\mathfrak{z}^{(n)}, g^{(n)}) = (h^{(n)} \cdot \mathfrak{z}^{(n)}, g^{(n)} \cdot (h^{(n)})^{-1}), \tag{4.3.12}$$

where defined. The second component of (4.3.12) corresponds to the usual right multiplication $R_h(g^{(n)}) = g^{(n)} \cdot (h^{(n)})^{-1}$ of the pseudo-group onto $\mathcal{G}^{(n)}$, [**54**]. The first component $h^{(n)} \cdot \mathfrak{z}^{(n)} = (s, h^{(n)} \cdot x^{(n)}, h^{(n)} \cdot u^{(n)}) = (s, X^{(n)}, U^{(n)})$ is the prolonged action of the pseudo-group $\mathcal{G}$ onto the jet space $\mathcal{J}^{(n)}$. Coordinate expressions for the prolonged action are obtained by differentiating the target coordinates $Z = (X, U)$ with respect to the computational variables $s$:

$$X^i_A = D^{a^1}_{s^1} \dots D^{a^p}_{s^p} X^i, \qquad U^\alpha_A = D^{a^1}_{s^1} \dots D^{a^p}_{s^p} U^\alpha, \tag{4.3.13}$$

where $A = (a^1, \dots, a^p)$. The expressions (4.3.13) are invariant under the *lifted action* (4.3.12) and these functions are called *lifted invariants.*

**Definition 4.3.6.** A *(right) moving frame* of order $n$ is a $\mathcal{G}$-equivariant section $\widehat{\rho}^{(n)}$ of the lifted bundle $\mathcal{B}^{(n)} \to \mathcal{J}^{(n)}$.

In local coordinates, the notation

$$\widehat{\rho}^{(n)}(\mathfrak{z}^{(n)}) = (\mathfrak{z}^{(n)}, \rho^{(n)}(\mathfrak{z}^{(n)}))$$

is used to denote an order $n$ right moving frame. Right equivariance means that for $g \in \mathcal{G}$

$$R_g \widehat{\rho}^{(n)}(\mathfrak{z}^{(n)}) = \widehat{\rho}^{(n)}(g^{(n)} \cdot \mathfrak{z}^{(n)}),$$

where defined.

**Definition 4.3.7.** Let

$$\mathcal{G}^{(n)}_{\mathfrak{z}^{(n)}} = \left\{ g^{(n)} \in \mathcal{G}^{(n)}|_{\mathfrak{z}} \, : \, g^{(n)} \cdot \mathfrak{z}^{(n)} = \mathfrak{z}^{(n)} \right\}$$

denote the *isotropy subgroup* of $\mathfrak{z}^{(n)} \in \mathcal{J}^{(n)}$. The pseudo-group $\mathcal{G}$ is said to act *freely* at $\mathfrak{z}^{(n)} \in \mathcal{J}^{(n)}$ if $\mathcal{G}^{(n)}_{\mathfrak{z}^{(n)}} = \{\mathbb{1}^{(n)}|_{\mathfrak{z}}\}$. The pseudo-group $\mathcal{G}$ is said to act *freely at order n* if it acts freely on an open subset $\mathcal{V}^{(n)} \subset \mathcal{J}^{(n)}$, called the set of *regular n-jets.*

**Theorem 4.3.8.** Suppose $\mathcal{G}$ acts freely on $\mathcal{V}^{(n)} \subset \mathcal{J}^{(n)}$, with its orbits forming a regular foliation. Then an $n^{\text{th}}$ order moving frame exists in a neighbourhood of $\mathfrak{z}^{(n)} \in \mathcal{V}^{(n)}$.

Once a pseudo-group acts freely, a result known as the *persistence of freeness*, [**55, 56**], guarantees that the action remains free under prolongation.

**Theorem 4.3.9.** If a Lie pseudo-group $\mathcal{G}$ acts freely at $\mathfrak{z}^{(n)}$, then it acts freely at any $\mathfrak{z}^{(k)} \in \mathcal{J}^{(k)}$, $k \geq n$, with $\pi^k_n(\mathfrak{z}^{(k)}) = \mathfrak{z}^{(n)}$.

**Remark 4.3.10.** Theorems 4.3.8 and 4.3.9 also hold when the pseudo-group action is locally free, meaning that the isotropy group $\mathcal{G}^{(n)}_{\mathfrak{z}^{(n)}}$ is a discrete subgroup of $\mathcal{G}^{(n)}\big|_{\mathfrak{z}}$.

An order $n \geq n^\star$ moving frame is constructed through a normalization procedure based on the choice of a cross-section $\mathcal{K}^{(n)} \subset \mathcal{V}^{(n)}$ to the pseudo-group orbits. The associated (locally defined) right moving frame section $\widehat{\rho}^{(n)} \colon \mathcal{V}^{(n)} \to \mathcal{B}^{(n)}$ is uniquely characterized by the condition that $\rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)} \in \mathcal{K}^{(n)}$. In coordinates, assuming that

$$\mathcal{K}^{(n)} = \{z_{i_1} = c_1, \ldots, z_{i_{r_n}} = c_{r_n} \ : \ r_n = \dim\, \mathcal{G}^{(n)}|_{\mathfrak{z}}\} \tag{4.3.14}$$

is a coordinate cross-section, the moving frame $\widehat{\rho}^{(n)}$ is obtained by solving the *normalization equations*

$$Z_{i_1}(s, x^{(n)}, u^{(n)}, g^{(n)}) = c_1, \qquad \ldots \qquad Z_{i_{r_n}}(s, x^{(n)}, u^{(n)}, g^{(n)}) = c_{r_n},$$

for the pseudo-group parameters $g^{(n)} = \rho^{(n)}(\mathfrak{z}^{(n)})$. As one increases the order from $n$ to $k > n$, a new cross-section $\mathcal{K}^{(k)} \subset \mathrm{J}^{(k)}$ must be selected. These cross-sections are required to be compatible meaning that $\pi^k_n(\mathcal{K}^{(k)}) = \mathcal{K}^{(n)}$ for all $k > n$. This in turn, implies the compatibility of the moving frames: $\widehat{\pi}^k_n \circ \widehat{\rho}^{(k)} = \widehat{\rho}^{(n)} \circ \pi^k_n$, where $\widehat{\pi}^k_n \colon \mathcal{B}^{(k)} \to \mathcal{B}^{(n)}$ is the standard projection.

**Proposition 4.3.11.** Let $\widehat{\rho}^{(n)}$ be an $n^{\text{th}}$ order right moving frame. The *normalized invariants*

$$(s, H^{(n)}, I^{(n)}) = \iota(s, x^{(n)}, u^{(n)}) = \rho^{(n)}(\mathfrak{z}^{(n)}) \cdot \mathfrak{z}^{(n)},$$

form a complete set of differential invariants of order $\leq n$.

**Example 4.3.12.** In this example we construct a moving frame for the pseudo-group (4.2.1). The computations for graphs of functions $(x, y, u(x, y))$ appear in [**54**]. In preparation for the next section we revisit the calculations using the computational variables $(s, t)$ so that $x = x(s, t)$, $y = y(s, t)$ and $u = u(s, t)$. To simplify the computations let

$$y = k\,t + y_0, \tag{4.3.15a}$$

where $k > 0$ and $y_0$ are constants, and assume that

$$x_t = 0. \tag{4.3.15b}$$

In other words, $x = x(s)$ is a function of the computational variable $s$. We note that the constraints (4.3.15) are invariant under the pseudo-group action (4.2.1). For the $y$ variable, this is straightforward as it is an invariant. The invariance of (4.3.15b) follows from the chain rule:

$$X_t = f_x\, x_t = 0 \qquad \text{when} \qquad x_t = 0.$$

The non-degeneracy condition (4.3.8) requires the invariant constraint $x_s \neq 0$ to be satisfied.

Up to order 2, the prolonged action is

$$\begin{gathered} S = s, \qquad T = t, \qquad Y = y, \qquad X = f(x), \qquad U = \frac{u}{f_x}, \\ X_s = f_x\, x_s, \qquad Y_t = k, \qquad U_s = \frac{u_s}{f_x} - \frac{u\, f_{xx}\, x_s}{f_x^2}, \qquad U_t = \frac{u_t}{f_x}, \\ X_{ss} = f_{xx}\, x_s^2 + f_x\, x_{ss}, \qquad Y_{tt} = 0, \qquad U_{tt} = \frac{u_{tt}}{u}, \qquad U_{st} = \frac{u_{st}}{f_x} - \frac{u_t\, f_{xx}\, x_s}{f_x^2}, \\ U_{ss} = \frac{u_{ss}}{f_x} + 2\frac{u\, f_{xx}^2\, x_s^2}{f_x^3} - 2\frac{u_s\, f_{xx}\, x_s}{f_x^2} - \frac{u\, f_{xxx}\, x_s^2}{f_x^2} - \frac{u\, f_{xx}\, x_{ss}}{f_x^2}. \end{gathered} \tag{4.3.16}$$

A cross-section to the prolonged action (4.3.16) and its prolongation is given by

$$\mathcal{K}^{(\infty)} = \{x = 0,\ u = 1,\ u_{s^k} = 0,\ k \geq 1\}. \tag{4.3.17}$$

Solving the normalization equations

$$X = 0, \qquad U = 1, \qquad U_{s^k} = 0, \qquad k \geq 1,$$

for the pseudo-group parameters $f, f_x, f_{xx}, \ldots$, we obtain the right moving frame

$$f = 0, \qquad f_x = u, \qquad f_{xx} = \frac{u_s}{x_s}, \qquad f_{xxx} = \frac{u_{ss}}{x_s^2} - \frac{u_s\, x_{ss}}{x_s^3}, \qquad \ldots .$$

In general,

$$f = 0, \qquad f_{x^{k+1}} = \left(\frac{D_s}{x_s}\right)^k u, \qquad k \geq 0. \tag{4.3.18}$$

Substituting the pseudo-group normalizations (4.3.18) into the prolonged action (4.3.16) yields the normalized differential invariants

$$\begin{gathered} \iota(s) = s, \qquad \iota(t) = t, \qquad \iota(y) = y, \qquad I_1 = \iota(x_s) = u\, x_s, \qquad \iota(y_t) = k, \\ J_{0,1} = \iota(u_t) = \frac{u_t}{u}, \qquad I_2 = \iota(x_{ss}) = u_s\, x_s + u\, x_{ss}, \qquad \iota(y_{tt}) = 0, \\ J_{0,2} = \iota(u_{tt}) = \frac{u_{tt}}{u}, \qquad J_{1,1} = \iota(u_{st}) = \frac{u\, u_{st} - u_t\, u_s}{u^2}. \end{gathered} \tag{4.3.19}$$

**Remark 4.3.13.** To transition between the expressions obtained in Example 4.3.12 and those appearing in [**54**], it suffices to use the chain rule. When (4.3.15) holds,

$$D_x = \frac{D_s}{x_s}, \qquad D_y = \frac{D_t}{k},$$

so that

$$u_x = \frac{u_s}{x_s}, \quad u_y = \frac{u_t}{k}, \quad u_{xx} = \frac{x_s\, u_{ss} - u_s\, x_{ss}}{x_s^3}, \quad u_{xy} = \frac{u_{st}}{k\, x_s}, \quad u_{yy} = \frac{u_{tt}}{k^2}, \quad \ldots . \tag{4.3.20}$$

The prolonged action on $u_x$, $u_y$, ..., can then be obtained by substituting (4.3.16) into (4.3.20). For example,

$$U_X = \frac{U_s}{X_s} = \left(\frac{u_s}{f_x} - \frac{u\, f_{xx}\, x_s}{f_x^2}\right)\frac{1}{f_x\, x_s} = \frac{u_x}{f_x^2} - \frac{u\, f_{xx}}{f_x^3}.$$

In the jet variables $z^{(\infty)} = (x, y, u^{(\infty)}) = (x, y, u, u_x, u_y, \ldots)$ a cross-section is given by, [**54**],

$$\overline{\mathcal{K}}^{(\infty)} = \{x = 0,\ u = 1,\ u_{x^k} = 0,\ k \geq 1\}, \tag{4.3.21}$$

and the corresponding moving frame is

$$f = 0, \qquad f_{x^{k+1}} = u_{x^k}, \qquad k \geq 0. \tag{4.3.22}$$

Expressing $u_{x^k}$ in terms of the derivatives $x_{s^k}$, $u_{s^k}$ using (4.3.20), one sees that (4.3.21) and (4.3.22) are equivalent to (4.3.17) and (4.3.18) in the computational variable framework. In the following, the cross-sections (4.3.17) and (4.3.21) (and the corresponding moving frames (4.3.18) and (4.3.22)) are said to be *equivalent*.

Not all cross-sections are equivalent. For example, instead of using the cross-section (4.3.17), it is also possible to choose the (non-minimal) cross-section

$$\widetilde{\mathcal{K}}^{(\infty)} = \{x = 0,\ x_s = 1,\ x_{s^{k+2}} = 0,\ k \geq 0\}. \tag{4.3.23}$$

Since (4.3.21) is not related to (4.3.23) by the substitutions (4.3.20), the cross-section (4.3.23) is said to be *inequivalent* to (4.3.21).

**Definition 4.3.14.** Let $\mathcal{G}^{(n)}$ be a Lie pseudo-group acting on $\mathrm{J}^{(n)}$ and $\mathcal{J}^{(n)}$. A cross-section $\mathcal{K}^{(n)} \subset \mathcal{J}^{(n)}$ is said to be *equivalent* with the cross-section $\overline{\mathcal{K}}^{(n)} \subset \mathrm{J}^{(n)}$ if the defining equation (4.3.14) of $\mathcal{K}^{(n)}$ are obtained from those of $\overline{\mathcal{K}}^{(n)}$ by expressing the submanifold jet $z^{(n)}$ in terms of $\mathfrak{z}^{(n)}$ using the relations (4.3.10).

## 4.4. Discrete pseudo-groups and moving frames

Let $M^{\times k}$ denote the $k$-fold Cartesian product of a manifold $M$. Discrete points in $M$ are labelled using the multi-index notation

$$z_N = (x_N, u_N), \qquad N = (n^1, \ldots, n^p) \in \mathbb{Z}^p. \tag{4.4.1}$$

The multi-index notation (4.4.1) can be related to the continuous theory of Section 4.3 in the following way. The multi-index $N = (n^1, \ldots, n^p) \in \mathbb{Z}^p \subset \mathbb{R}^p$ can be thought as sampling the computational variables $s = (s^1, \ldots, s^p) \in \mathbb{R}^p$ on a unit hypercube grid. Thus, the notation $z_N = z(N)$ can be understood as sampling a submanifold $S \subset M$ parameterized by $z(s) = (x(s), u(s))$ at the integer points $N \in \mathbb{Z}^p$.

To mimic the continuous theory of moving frames in the finite difference setting, a discrete counterpart to the submanifold jet space $\mathcal{J}^{(n)}$ is introduced.

**Definition 4.4.1.** Let $M$ be a manifold with local coordinate system $z = (x, u)$. The $k$-fold *joint product* of $M$ is a subset of the $k$-fold Cartesian product $M^{\times k}$ given by

$$M^{\diamond k} = \{(z_{N_1}, \ldots, z_{N_k}) \,|\, z_{N_i} \neq z_{N_j} \text{ for all } i \neq j\} \subset M^{\times k}.$$

**Definition 4.4.2.** The $n^{\text{th}}$ order *forward discrete jet* at the multi-index $N$ is the point

$$\mathfrak{z}_N^{[n]} = (N, \ldots\, z_{N+K}\, \ldots), \tag{4.4.2}$$

where $(\ldots\, z_{N+K}\, \ldots) \in M^{\diamond d_n}$ with

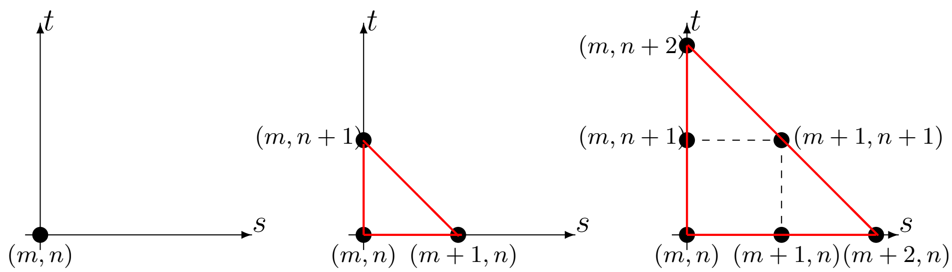
$$d_n = m\binom{p+n}{n}, \qquad m = \dim M,$$

and $K = (k^1, \ldots, k^p)$ is a non-negative multi-index of order $0 \leq \#K \leq n$.

In dimension 2, when $N = (m, n)$, Figure 4.2 shows the multi-indices contained in a forward discrete jet or order $\leq 2$. In general, the multi-indices included in $\mathfrak{z}_{m,n}^{[k]}$ are those contained in the interior and boundary of the right isosceles triangle with vertices at $(m, n)$, $(m+k, n)$ and $(m, n+k)$.

**Definition 4.4.3.** The $n^{\text{th}}$ order *forward joint jet space* $\mathcal{J}^{[n]}$ is the collection of forward discrete jets (4.4.2):

$$\mathcal{J}^{[n]} = \bigcup_{N \in \mathbb{Z}^p} \mathfrak{z}_N^{[n]}.$$




(a) $k=0$ (b) $k=1$ (c) $k=2$

FIG. 4.2. Multi-indices occuring in $\mathfrak{z}^{[k]}_{m,n} \in \mathcal{J}^{[k]}$ for $k = 0, 1, 2$.

For $k > n$, $\pi^k_n \colon \mathcal{J}^{[k]} \to \mathcal{J}^{[n]}$ will denote the projection obtained by truncating $\mathfrak{z}^{[k]}_N = (N, \ldots\ z_{N+K}\ \ldots)$, $0 \leq \#K \leq k$, to

$$\pi^k_n(\mathfrak{z}^{[k]}_N) = \mathfrak{z}^{[n]}_N = (N, \ldots\ z_{N+K}\ \ldots), \qquad 0 \leq \#K \leq n.$$

Let us explain how $\mathcal{J}^{[n]}$ can be understood as a discrete representation of the submanifold jet space $\mathcal{J}^{(n)}$. For this, let $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)$ be the $i^{\text{th}}$ element of the standard orthonormal basis of $\mathbb{R}^p$, and let

$$S_i(N) = N + e_i, \qquad i = 1, \ldots, p,$$

denote the forward shift operator in the $i^{\text{th}}$ component. Then, on a unit hypercube grid in the computational variables, the derivative operators $D_{s^i}$ can be approximated by the forward difference

$$D_{s^i} \sim \Delta_i = S_i - \mathbb{1}, \qquad i = 1, \ldots p,$$

where $\mathbb{1}(N) = N$ is the identity map. Then, for a non-negative multi-index $K = (k^1, \ldots, k^p)$,

$$z^N_{s^K} = \Delta_1^{k_1} \cdots \Delta_p^{k_p}(z_N) \tag{4.4.3}$$

is a forward difference approximation of the derivative $z_{s^K}$ at the point $s = N$. Making the change of variables $z_{N+K} \mapsto z^N_{s^K}$, we have that

$$\mathfrak{z}^{[n]}_N \simeq (N, \dots z^N_{s^K} \dots) = (N, \dots x^N_{s^K} \dots u^N_{s^K} \dots), \qquad 0 \leq \#K \leq n,$$

is a finite difference approximation of the submanifold jet $(s, x^{(n)}, u^{(n)})$ at the point $s = N$ on a unit hypercube grid. In this sense, $\mathfrak{z}^{[n]}_N$ can be thought as a discrete counterpart to the submanifold jet $\mathfrak{z}^{(n)} = (N, x^{(n)}, u^{(n)})$ in the computational variable formalism, [**28**].

**Remark 4.4.4.** In (4.4.3) and elsewhere, the usual derivative notation is supplemented by a superscript to denote (forward) discrete derivatives. The superscript indicates where the derivative is evaluated.

**Remark 4.4.5.** It is also possible to introduce a backward discrete jet space by introducing the backward differences

$$\nabla_i = \mathbb{1} - S^-_i, \qquad \text{where} \qquad S^-_i(N) = N - e_i.$$

For numerical purposes, it might be preferable to consider symmetric discrete jets, but to simplify the exposition we restrict ourself to forward differences. All constructions can be adapted to these alternative settings.

Now, assume that the discrete counterpart of the non-degeneracy condition (4.3.8) holds. Namely,

$$\det\,(\Delta_j(x^i_N)) \neq 0. \tag{4.4.4}$$

Then, discrete approximations $u^{\alpha;N}_{x^J}$ of the derivatives $u^\alpha_{x^J}$ can be obtained as follows:

(1) compute the expressions (4.3.10),

(2) replace the derivatives $D_{s^i}$ by the difference operators $\Delta_i$.

Since the independent variables $x^i_N$ do not have to form a rectangular grid, the finite difference approximations $u^{\alpha;N}_{x^J}$ will hold on any admissible mesh. Having these expressions will be important as below a Lie pseudo-group will act on $z_N = (x_N, u_N)$ and the expressions for $u^{\alpha;N}_{x^J}$ need to hold on general meshes, [**22, 40, 63**].

Using the approximations $u^{\alpha;N}_{x^J}$, a finite difference approximation of the jet space $\mathrm{J}^{(n)}$ is given by

$$\mathrm{J}^{(n)} \sim \mathrm{J}^{[n]} = \bigcup_{N\in\mathbb{Z}^p} (x_N, \ldots\, u^{\alpha;N}_{x^J}\, \ldots), \qquad 0 \le \#J \le n.$$

**Example 4.4.6.** To illustrate the above discussion, we consider the case of two independent variables $(x, y)$ and one dependent variable $u(x, y)$. Introducing the computational variables $(s, t) \in \mathbb{R}^2$ so that $x = x(s, t)$ and $y = y(s, t)$, the implicit total derivative operators (4.3.9) are

$$D_x = \frac{y_t\, D_s - y_s\, D_t}{x_s\, y_t - y_s\, x_t}, \qquad D_y = \frac{x_s\, D_t - x_t\, D_s}{x_s\, y_t - y_s\, x_t}, \tag{4.4.5}$$

with $x_s\, y_t - y_s\, x_t \neq 0$. Applying (4.4.5) to the dependent variable $u$ yields

$$u_x = D_x\, u = \frac{y_t\, u_s - y_s\, u_t}{x_s\, y_t - y_s\, x_t} \qquad \text{and} \qquad u_y = D_y\, u = \frac{x_s\, u_t - x_t\, u_s}{x_s\, y_t - y_s\, x_t}. \tag{4.4.6}$$

Using the multi-index $N = (m, n) \in \mathbb{Z}^2 \subset \mathbb{R}^2$ to sample the computational variables $(s, t)$ at integer values and introducing the shift operators

$$S_1(m, n) = (m + 1, n), \qquad S_2(m, n) = (m, n + 1),$$

and the difference operators

$$D_s \sim \Delta = S_1 - \mathbb{1}, \qquad D_t \sim \delta = S_2 - \mathbb{1}, \tag{4.4.7}$$

finite difference approximations of the first order partial derivatives (4.4.6) are given by

$$u^{m,n}_x = \frac{\delta y_{m,n}\, \Delta u_{m,n} - \Delta y_{m,n}\, \delta u_{m,n}}{\Delta x_{m,n}\, \delta y_{m,n} - \Delta y_{m,n}\, \delta x_{m,n}}, \qquad u^{m,n}_y = \frac{\Delta x_{m,n}\, \delta u_{m,n} - \delta x_{m,n}\, \Delta u_{m,n}}{\Delta x_{m,n}\, \delta y_{m,n} - \Delta y_{m,n} \delta x_{m,n}}, \tag{4.4.8}$$

provided $\Delta x_{m,n}\, \delta y_{m,n} - \Delta y_{m,n}\, \delta x_{m,n} \neq 0$.

The expressions (4.4.6) and their finite difference approximations (4.4.8) can be simplified if constraints on the functions $x(s,t)$ and $y(s,t)$ are imposed. For example, in Example 4.4.9 we will impose the constraints

$$x_t = 0 \qquad \text{and} \qquad y_{tt} = 0, \tag{4.4.9}$$

so that $x = x(s)$ and $y = t\, f(s) + g(s)$, with $f(s) \cdot x'(s) \neq 0$. The operators (4.4.5) then reduce to

$$D_x = \frac{y_t\; D_s - y_s\, D_t}{x_s\, y_t}, \qquad D_y = \frac{D_t}{y_t}, \tag{4.4.10}$$

and

$$\begin{gathered} u_x = \frac{y_t\, u_s - y_s\, u_t}{x_s\, y_t}, \qquad u_y = \frac{u_t}{y_t}, \qquad u_{yy} = \frac{u_{tt}}{y_t^2}, \qquad u_{xy} = \frac{y_t\, u_{st} - y_{st}\, u_t - y_s\, u_{tt}}{x_s\, y_t^2}, \\ u_{xx} = \frac{1}{x_s}\left[\frac{y_{st}\, u_s + y_t\, u_{ss} - y_{ss}\, u_t - y_s\, u_{st} - (x_{ss}\, y_t + x_s\, y_{st}) u_x}{x_s\, y_t} - y_s\, u_{xy}\right], \\ u_{yyy} = \frac{u_{ttt}}{y_t^3}, \qquad u_{xyy} = \frac{y_t\, u_{stt} - 2u_{tt}\, y_{st} - y_s\, u_{ttt}}{x_s\, y_t^3}, \qquad \ldots . \end{gathered} \tag{4.4.11}$$

At the discrete level the differential constraints (4.4.9) are replaced by

$$\delta x_{m,n} = 0 \qquad \text{and} \qquad \delta^2 y_{m,n} = \delta y_{m,n+1} - \delta y_{m,n} = y_{m,n+2} - 2y_{m,n+1} + y_{m,n} = 0.$$

This implies that $x_{m,n} = x_m$ is independent of the index $n$ while $y_{m,n} = n\, f(m) + g(m)$, with $\Delta x_m\, \delta y_{m,n} = (x_{m+1} - x_m) \cdot f(m) \neq 0$. Making the substitutions (4.4.7), the expressions (4.4.11) are approximated by

$$\begin{aligned} u_y^{m,n} &= \frac{\delta u_{m,n}}{\delta y_{m,n}}, & u_x^{m,n} &= \frac{\delta u_{m,n}\, \Delta u_{m,n} - \Delta y_{m,n}\, \delta u_{m,n}}{\Delta x_m\, \delta y_{m,n}}, \\ u_{yy}^{m,n} &= \frac{\delta^2 u_{m,n}}{(\delta y_{m,n})^2}, & u_{xy}^{m,n} &= \frac{\delta y_{m,n}\, \Delta \delta u_{m,n} - \Delta \delta y_{m,n}\, \Delta u_{m,n} - \Delta y_{m,n}\, \delta^2 u_{m,n}}{\Delta x_m\, (\delta y_{m,n})^2}, \\ u_{yyy}^{m,n} &= \delta^3 u_{m,n} (\delta y_{m,n})^3, & u_{xyy}^{m,n} &= \frac{\delta y_{m,n}\, \Delta \delta^2 u_{m,n} - 2\delta^2 u_{m,n}\, \Delta \delta y_{m,n} - \Delta y_{m,n}\, \delta^3 u_{m,n}}{\Delta x_m (\delta y_{m,n})^3}. \end{aligned} \tag{4.4.12}$$

We are now interested in the induced action of a Lie pseudo-group on discrete points.

**Definition 4.4.7.** Given a Lie pseudo-group $\mathcal{G}$ acting on $M$, the *pseudo-group product* action on the $k$-fold Cartesian product $M^{\times k}$ is

$$(g \cdot z_{N_1}, \ldots, g \cdot z_{N_k}), \qquad g \in \mathcal{G}, \tag{4.4.13}$$

provided the points $z_{N_1}, \ldots, z_{N_k} \in \operatorname{dom} g$.

**Remark 4.4.8.** The nature of the product action (4.4.13) depends on the type of the Lie pseudo-group $\mathcal{G}$. If the Lie pseudo-group $\mathcal{G}$ is of infinite type, its $k$-fold product action is no longer a Lie pseudo-group as it is not possible to encapsulate into a system of differential equations the requirement that the same diffeomorphism should act on different points. In this case, the product action only satisfies the defining properties of a pseudo-group. On the other hand, the $k$-fold product action of a Lie pseudo-group of finite type, i.e. a local Lie group action, remains a Lie pseudo-group of finite type. Another important distinction between pseudo-groups of finite and infinite types occurs when more copies of the manifold $M$ are appended to the Cartesian product $M^{\times k}$. For pseudo-groups of infinite type, when a new copy of $M$ is added, new pseudo-group parameters will occur in the product action while this is not the case for pseudo-groups of finite type.

As shown in Example 4.2.1, no joint invariant of the product action (4.2.5) can approximate the differential invariant (4.2.2). This is not peculiar to this pseudo-group and another instance is given in Example 4.4.21. To address this lack of joint invariants, we propose to discretize the product pseudo-group action, replacing derivatives by finite difference approximations. Before stating the general theory, our proposed idea is applied to the product pseudo-group (4.2.5).

**Example 4.4.9.** On the rectangular grid

$$\delta x_{m,n} = x_{m,n+1} - x_{m,n} = 0, \qquad y_n = k\,n + y_0,$$

a suitable discretization of the product pseudo-group action (4.2.5) is obtained by approximating the first order derivative $f_x(x_m)$ by the forward difference

$$f_x(x_m) \sim f_x^m = \frac{\Delta f_m}{\Delta x_m} = \frac{f_{m+1} - f_m}{x_{m+1} - x_m} \quad \text{where} \quad f_{m+j} = f(x_{m+j}), \tag{4.4.14}$$

to give the discretized action

$$\mathcal{G}_d\colon \qquad X_m = f_m, \qquad Y_n = y_n, \qquad U_{m,n} = \frac{u_{m,n}}{f_x^m}. \tag{4.4.15}$$

The subscript $d$ is added to $\mathcal{G}$ to indicate that the pseudo-group action has been discretized. For (4.4.15) to be a legitimate discretization it must satisfy the properties of an action. These are readily seen to be satisfied except maybe for closure under composition. To this end, let

$$\widetilde{X}_m = \widetilde{f}_m = \widetilde{f}(X_m), \qquad \widetilde{Y}_n = Y_n = y_n, \qquad \widetilde{U}_{m,n} = \frac{U_{m,n}}{\widetilde{f}_X^m},$$

be a second discretized transformation. Then $\widetilde{X}_m = \widetilde{f} \circ f(x_m)$, and

$$\begin{aligned} \widetilde{U}_{m,n} = U_{m,n} \cdot \frac{\Delta X_m}{\Delta[\widetilde{f}(X_m)]} &= u_{m,n} \cdot \frac{\Delta x_m}{\Delta[f(x_m)]} \cdot \frac{\Delta[f(x_m)]}{\Delta[\widetilde{f} \circ f(x_m)]} \\ &= u_{m,n} \cdot \frac{\Delta x_m}{\Delta[\widetilde{f} \circ f(x_m)]} = \frac{u_{m,n}}{(\widetilde{f} \circ f)_x^m}, \end{aligned}$$

showing that (4.4.15) is closed under composition.

The approximation (4.4.14) is not unique. Any other discretization preserving the group action properties is acceptable. For example, the approximation (4.4.14) could be replaced by the backward difference

$$f_x(x_m) \sim \frac{f_m - f_{m-1}}{x_m - x_{m-1}}.$$

On the other hand, (4.4.15) is not closed under composition if the centred approximation

$$f_x(x_m) \sim \frac{1}{2}\left[\frac{\Delta f_m}{\Delta x_m} + \frac{\Delta f_{m-1}}{\Delta x_{m-1}}\right]$$

is considered.

At the infinitesimal level, the discretized action (4.4.15) is generated by the vector field

$$\mathbf{v}_a = a_m \frac{\partial}{\partial x_m} - u_{m,n}\, a_x^m \frac{\partial}{\partial u_{m,n}}, \tag{4.4.16}$$

where

$$a_m = a(x_m) \qquad \text{and} \qquad a_x^m = \frac{a_{m+1} - a_m}{x_{m+1} - x_m}.$$

To compute the Lie algebra structure of (4.4.16), one would use the standard prolongation, [**40**],

$$\mathbf{pr}\,\mathbf{v}_a = \sum_m a_m \frac{\partial}{\partial x_m} - \sum_{m,n} u_{m,n}\, a_x^m \frac{\partial}{\partial u_{m,n}}$$

and define the Lie bracket $[\mathbf{v}_a, \mathbf{v}_b]$ of two infinitesimal generators to be the vector field satisfying

$$\mathbf{pr}\,[\mathbf{v}_a, \mathbf{v}_b] := \mathbf{pr}\,\mathbf{v}_a \circ \mathbf{pr}\,\mathbf{v}_b - \mathbf{pr}\,\mathbf{v}_b \circ \mathbf{pr}\,\mathbf{v}_a.$$

For two infinitesimal generators of the form (4.4.16), we obtain the expected commutation relation

$$[\mathbf{v}_a, \mathbf{v}_b] = \mathbf{v}_{ab'-ba'}.$$

**Remark 4.4.10.** By introducing the approximation (4.4.14), the discretized action (4.4.15) is no longer local as the approximation (4.4.14) introduces the extra independent variable $x_{m+1}$ into the action at $(x_m, y_n, u_{m,n})$. This type of non-local discrete transformations is reminiscent of transformations obtained when considering discrete generalized symmetries, [**40**]. Similar pseudo-group discretization also recently appeared in a discrete version of Noether's Second Theorem, [**29**].

Given an admissible discrete pseudo-group action, it is possible to implement the moving frame method in a fashion similar to the continuous setting. In the continuous theory, the jets of functions occurring in the prolonged action play the role of the pseudo-group parameters. In the discrete case, the functions evaluated at distinct points will play the role of the pseudo-group parameters.

**Example 4.4.11.** At the point $(x_m, y_n, u_{m,n})$, the discrete pseudo-group action

$$X_m = f_m = f(x_m), \qquad Y_n = y_n, \qquad U_{m,n} = u_{m,n} \cdot \frac{x_{m+1} - x_m}{f_{m+1} - f_m}$$

involves the pseudo-group parameters $g_{m,n} = (f_m, f_{m+1})$.

In the following, the pseudo-group parameters occurring in the discrete pseudo-group action at $z_N$ is denoted $g_N$. To approximate the $n^{\text{th}}$ order lifted bundle (4.3.11) we introduce the $n^{\text{th}}$ order *forward joint lifted bundle* $\mathcal{B}^{[n]}$ parameterized by $(\mathfrak{z}_N^{[n]}, g_N^{[n]})$, where

$$g_N^{[n]} = (\ldots\, g_{N+K}\, \ldots), \qquad 0 \leq \#K \leq n.$$

The fibre of the $n^{\text{th}}$ order forward joint lifted bundle $\mathcal{B}^{[n]}$ at $\mathfrak{z}_N^{[n]}$ is denoted $\mathcal{G}_N^{[n]}$. The discretized pseudo-group $\mathcal{G}_d$ acts on $\mathcal{B}^{[n]}$ by right multiplication

$$R_{h_N}(\mathfrak{z}_N^{[n]}, g_N^{[n]}) = (h_N^{[n]} \cdot \mathfrak{z}_N^{[n]}, (g \cdot h^{-1})^{[n]}|_{h_N^{[n]} \cdot \mathfrak{z}_N^{[n]}}).$$

**Definition 4.4.12.** Let $\mathcal{G}_d$ be a discretized Lie pseudo-group acting on the $n^{\text{th}}$ order joint lifted bundle $\mathcal{B}^{[n]}$. An order $n$ (right) *joint moving frame* is a $\mathcal{G}_d$-equivariant section of the order $n$ joint lifted bundle $\mathcal{B}^{[n]}$:

$$\widehat{\rho}^{[n]}(\mathfrak{z}_N^{[n]}) = (\mathfrak{z}_N^{[n]},\, \rho^{[n]}(\mathfrak{z}_N^{[n]})).$$

Right equivariance means that

$$R_{g_N}\widehat{\rho}^{[n]}(\mathfrak{z}_N^{[n]}) = \widehat{\rho}^{[n]}(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}).$$

As in the continuous setting, a moving frame exists on (an open set of) the $n^{\text{th}}$ order joint bundle $\mathcal{J}^{[n]}$ if the action is free and regular.

**Definition 4.4.13.** A discretized Lie pseudo-group $\mathcal{G}_d$ acts freely at $\mathfrak{z}_N^{[n]}$ if the isotropy group

$$\mathcal{G}^{[n]}_{N;\mathfrak{z}_N^{[n]}} = \{g_N^{[n]} \,:\, g_N^{[n]} \cdot \mathfrak{z}_N^{[n]} = \mathfrak{z}_N^{[n]}\} = \{\mathbb{1}_N^{[n]}\}, \tag{4.4.17}$$

where $\mathbb{1}_N^{[n]}$ is the discrete identity transformation at $\mathfrak{z}_N^{[n]}$.

**Example 4.4.14.** For the discretized pseudo-group (4.4.15), the isotropy condition $\mathfrak{g}^{[0]}_{m,n} \cdot \mathfrak{z}^{[0]}_{m,n} = \mathfrak{z}^{[0]}_{m,n}$ is

$$x_m = f_m, \qquad y_n = y_n, \qquad u_{m,n} = \frac{u_{m,n}}{f_x^m}$$

which requires

$$f_m = x_m, \qquad f_{m+1} = x_{m+1}.$$

In general, the isotropy condition $\mathfrak{g}^{[k]}_{m,n} \cdot \mathfrak{z}^{[k]}_{m,n} = \mathfrak{z}^{[k]}_{m,n}$ yields

$$f_{m+\ell} = x_{m+\ell}, \qquad \ell = 0, \ldots, k+1.$$

Provided the discrete product pseudo-group action is free and regular, a joint moving frame is constructed through a normalization procedure similar to the continuous case. Let $\mathcal{K}^{[n]} = \{z_{i_1} = c_1, \ldots, z_{i_{r_n}} = c_{r_n}\} \subset \mathcal{J}^{[n]}$ be a coordinate cross-section, then the corresponding joint moving frame $\widehat{\rho}^{[n]}$ is obtained by solving the normalization equations

$$Z_{i_1}(\mathfrak{z}_N^{[n]}, g_N^{[n]}) = c_1, \qquad \ldots \qquad Z_{i_{r_n}}(\mathfrak{z}_N^{[n]}, g_N^{[n]}) = c_{r_n}$$

for the pseudo-group parameters $g_N^{[n]} = \rho^{[n]}(\mathfrak{z}_N^{[n]})$. For $k > n$, the cross-sections are required to be compatible, that is $\pi_n^k(\mathcal{K}^{[k]}) = \mathcal{K}^{[n]}$. The corresponding moving frames are then compatible $\widehat{\pi}_n^k \circ \widehat{\rho}^{[n]} = \widehat{\rho}^{[n]} \circ \pi_n^k$. Here $\widehat{\pi}_n^k \colon \mathcal{B}^{[k]} \to \mathcal{B}^{[n]}$ is the standard projection obtained by truncation. A discrete analogue of Theorem 4.3.9 also holds.

**Theorem 4.4.15.** Let $\mathcal{G}_d$ be the discretization of a Lie pseudo-group and assume it acts freely at $\mathfrak{z}_N^{[n]}$ for any $N \in \mathbb{Z}^p$. Then for $k > n$, $\mathcal{G}_d$ acts freely at $\mathfrak{z}_N^{[k]}$.

**Remark 4.4.16.** Before proving Theorem 4.4.15 in general, it is instructive to consider a low dimensional example. In two dimensions, assume the discretized action is free at $\mathfrak{z}_{m,n}^{[2]}$. Our goal is to show that it remains free at $\mathfrak{z}_{m,n}^{[3]}$. In Figure 4.3(a), the multi-indices contained in $\mathfrak{z}_{m,n}^{[3]}$ are displayed. Figures 4.3(c-d) show that sitting inside $\mathfrak{z}_{m,n}^{[3]}$ are the order 2 discrete jets

$$\mathfrak{z}_{m,n}^{[2]}, \qquad \mathfrak{z}_{m+1,n}^{[2]}, \qquad \mathfrak{z}_{m,n+1}^{[2]}.$$

Since these three order 2 jets cover $\mathfrak{z}_{m,n}^{[3]}$,

$$\mathfrak{z}_{m,n}^{[3]} \simeq (\mathfrak{z}_{m,n}^{[2]}, \mathfrak{z}_{m+1,n}^{[2]}, \mathfrak{z}_{m,n+1}^{[2]}). \tag{4.4.18a}$$

Similarly, at the pseudo-group level

$$g_{m,n}^{[3]} \simeq (g_{m,n}^{[2]}, g_{m+1,n}^{[2]}, g_{m,n+1}^{[2]}). \tag{4.4.18b}$$

Next, a pseudo-group transformation $g_{m,n}^{[3]} \in \mathcal{G}_{m,n}^{[3]}$ keeps $\mathfrak{z}_{m,n}^{[3]}$ fixed if and only if it keeps $\mathfrak{z}_{m,n}^{[2]}$, $\mathfrak{z}_{m+1,n}^{[2]}$, $\mathfrak{z}_{m,n+1}^{[2]}$ fixed simultaneously. That is

$$\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[3]}_{m,n}} = \mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m,n}} \cap \mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m+1,n}} \cap \mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m+1,n}}, \tag{4.4.19}$$

where

$$\begin{aligned}
\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m,n}} &= \{g^{[3]}_{m,n} \;:\; g^{[3]}_{m,n} \cdot \mathfrak{z}^{[2]}_{m,n} = g^{[2]}_{m,n} \cdot \mathfrak{z}^{[2]}_{m,n} = \mathfrak{z}^{[2]}_{m,n}\}, \\
\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m+1,n}} &= \{g^{[3]}_{m,n} \;:\; g^{[3]}_{m,n} \cdot \mathfrak{z}^{[2]}_{m+1,n} = g^{[2]}_{m+1,n} \cdot \mathfrak{z}^{[2]}_{m+1,n} = \mathfrak{z}^{[2]}_{m+1,n}\}, \\
\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m,n+1}} &= \{g^{[3]}_{m,n} \;:\; g^{[3]}_{m,n} \cdot \mathfrak{z}^{[2]}_{m,n+1} = g^{[2]}_{m,n+1} \cdot \mathfrak{z}^{[2]}_{m,n+1} = \mathfrak{z}^{[2]}_{m,n+1}\}.
\end{aligned}$$

By assumption

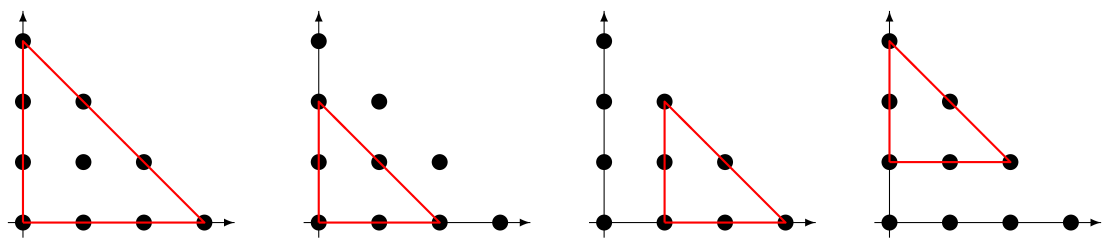
$$\mathcal{G}^{[2]}_{m,n;\mathfrak{z}^{[2]}_{m,n}} = \{\mathbb{1}^{[2]}_{m,n}\}, \qquad \mathcal{G}^{[2]}_{m+1,n;\mathfrak{z}^{[2]}_{m+1,n}} = \{\mathbb{1}^{[2]}_{m+1,n}\}, \qquad \mathcal{G}^{[2]}_{m,n+1;\mathfrak{z}^{[2]}_{m,n+1}} = \{\mathbb{1}^{[2]}_{m,n+1}\},$$

and it follows that

$$\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m,n}} \simeq \{(\mathbb{1}^{[2]}_{m,n}, *, *)\}, \qquad \mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m+1,n}} \simeq \{(*, \mathbb{1}^{[2]}_{m+1,n}, *)\},$$
$$\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[2]}_{m,n+1}} \simeq \{(*, *, \mathbb{1}^{[2]}_{m,n+1})\}, \tag{4.4.20}$$

under the isomorphism (4.4.18). The exact expressions for $*$ will depend on the particular pseudo-group action. Combining (4.4.19) and (4.4.20), we conclude that

$$\mathcal{G}^{[3]}_{m,n;\mathfrak{z}^{[3]}_{m,n}} \simeq \{(\mathbb{1}^{[2]}_{m,n}, \mathbb{1}^{[2]}_{m+1,n}, \mathbb{1}^{[2]}_{m,n+1})\} \simeq \{\mathbb{1}^{[3]}_{m,n}\}.$$



(a) $\mathfrak{z}^{[3]}_{m,n}$ (b) $\mathfrak{z}^{[2]}_{m,n}$ (c) $\mathfrak{z}^{[2]}_{m+1,n}$ (d) $\mathfrak{z}^{[2]}_{m,n+1}$

FIG. 4.3. Forward discrete jets of order 2 contained in $\mathfrak{z}^{[3]}_{m,n}$.

PROOF. To prove Theorem 4.4.15, it suffices to consider the case when $k = n+1$ and proceed as in the 2-dimensional example above. First,

$$\mathfrak{z}^{[n+1]}_{N} \simeq (\ldots\ \mathfrak{z}^{[n]}_{N+e_i}\ \ldots), \qquad i = 1, \ldots, p.$$

Next, since by assumption

$$\mathcal{G}^{[n]}_{N+e_i;z^{[n]}_{N+e_i}} = \{\mathbb{1}^{[n]}_{N+e_i}\}, \qquad i = 1, \ldots, p,$$

one has that

$$\begin{aligned}\mathcal{G}^{[n+1]}_{N;\mathfrak{z}^{[n]}_{N+e_i}} &= \{g^{[n+1]}_N \,:\, g^{[n+1]}_N \cdot \mathfrak{z}^{[n]}_{N+e_i} = g^{[n]}_{N+e_i} \cdot \mathfrak{z}^{[n]}_{N+e_i} = \mathfrak{z}^{[n]}_{N+e_i}\} \\ &\simeq \{(\ldots, *, \ldots, \mathbb{1}^{[n]}_{N+e_i}, \ldots, *, \ldots)\},\end{aligned}$$

and

$$\mathcal{G}^{[n+1]}_{N;\mathfrak{z}^{[n+1]}_N} = \bigcap_{i=1}^{p} \mathcal{G}^{[n+1]}_{N;\mathfrak{z}^{[n]}_{N+e_i}} = \{\mathbb{1}^{[n+1]}_N\}.$$

□

**Definition 4.4.17.** A function $I(\mathfrak{z}^{[n]}_N)\colon \mathcal{J}^{[n]} \to \mathbb{R}$ is a *joint invariant* if

$$I(g^{[n]}_N \cdot \mathfrak{z}^{[n]}_N) = I(\mathfrak{z}^{[n]}_N), \qquad g^{[n]}_N \in \mathcal{G}^{[n]}_N,$$

whenever the discrete product action is defined.

**Definition 4.4.18.** Let $\widehat{\rho}^{[n]}(\mathfrak{z}^{[n]}_N)$ be an order $n$ joint moving frame. The *invariantization* of a function $F(\mathfrak{z}^{[n]}_N)$ is the joint invariant

$$\iota(F)(\mathfrak{z}^{[n]}_N) = F(\rho^{[n]}(\mathfrak{z}^{[n]}_N) \cdot \mathfrak{z}^{[n]}_N). \tag{4.4.21}$$

Of particular interest to us is the invariantization of the discrete derivatives $u^{\alpha;N}_{x^J}$:

$$I^{\alpha;N}_J = \iota(u^{\alpha;N}_{x^J}), \qquad \alpha = 1, \ldots, q, \qquad \#J \geq 0. \tag{4.4.22}$$

We say that the cross-section $\mathcal{K}^{[n]}$ used to construct a joint moving frame $\widehat{\rho}^{[n]}$ is *consistent* with the cross-section $\mathcal{K}^{(n)}$ used to construct a (continuous) moving frame $\widehat{\rho}^{(n)}$ if, in the continuous limit, $\mathcal{K}^{[n]}$ converges to $\mathcal{K}^{(n)}$. For consistent cross-sections, since the discretized pseudo-group action $\mathcal{G}_d$ converges to the Lie pseudo-group $\mathcal{G}$ in the continuous limit, the discrete invariants (4.4.22) will converge to the differential invariants $I^\alpha_J = \iota(u^\alpha_{x^J})$:

$$\iota(u^{\alpha;N}_{x^J}) = I^{\alpha;N}_J \to I^\alpha_J = \iota(u^\alpha_{x^J}).$$

**Example 4.4.19.** In this example, a joint moving frame for the discretized pseudo-group action (4.4.15) is constructed. First, a cross-section is given by

$$\mathcal{K}^{[\infty]} = \{x_m = 0,\ u_{m+k,n} = 1,\ k \in \mathbb{N}\}. \tag{4.4.23}$$

Written differently, the cross-section is equivalent to

$$x_m = 0, \qquad u_{m,n} = 1, \qquad \Delta^k(u_{m,n}) = 0, \qquad k = 1, 2, \ldots, \tag{4.4.24}$$

which is an approximation of (4.3.17) on a unit square mesh in the computational variables $(s,t)$. Hence, (4.4.23) is consistent with the cross-section (4.3.17) used in the continuous setting. Solving the normalization equations

$$0 = X_m = f_m, \qquad 1 = U_{m+k,n} = \frac{u_{m+k,n}}{f_x^{m+k}} = u_{m+k,n} \cdot \frac{\Delta x_{m+k}}{\Delta f_{m+k}},$$

for the pseudo-group parameters $f_{m+k}$, $k \geq 0$, produces the (forward) joint moving frame

$$f_m = 0, \qquad f_{m+k} = \sum_{l=1}^{k} u_{m+l-1,n}\, \Delta x_{m+l-1}, \qquad k = 1, 2, 3, \ldots. \tag{4.4.25}$$

Applying the invariantization map (4.4.21) to the discrete variables $x_{m+k}$, $y_{n+l}$, $u_{m+k,n+l}$, we obtain the normalized joint invariants

$$\begin{gathered} \iota(x_{m+k}) = (\rho^{[\infty]})^* f_{m+k} = \begin{cases} 0 & k = 0, \\ \displaystyle\sum_{l=1}^{k} u_{m+l-1,n}\, \Delta x_{m+l-1} & k = 1, 2, 3, \ldots, \end{cases} \\ \iota(y_{n+l}) = y_{n+l}, \qquad \iota(u_{m+k,n+l}) = \frac{u_{m+k,n+l}}{(\rho^{[\infty]})^* f_x^{m+k}} = \frac{u_{m+k,n+l}}{u_{m+k,n}}, \qquad k, l = 0, 1, 2, \ldots. \end{gathered} \tag{4.4.26}$$

Alternatively, invariantizing the forward differences in $x_m$, $y_n$, $u_{m,n}$ yields the joint invariants

$$\iota(y_n) = y_n, \quad I_1^d = \iota(\Delta x_m) = u_{m,n}\, \Delta x_m, \quad \iota(\delta y_n) = k,$$
$$J_{0,1}^d = \iota(\delta u_{m,n}) = \frac{\delta u_{m,n}}{u_{m,n}}, \quad I_2^d = \iota(\Delta^2 x_m) = \Delta u_{m,n}\, \Delta x_m + u_{m,n}\, \Delta^2 x_m, \quad \iota(\delta^2 y_n) = 0,$$
$$J_{0,2}^d = \iota(\delta^2 u_{m,n}) = \frac{\delta^2 u_{m,n}}{u_{m,n}}, \quad J_{1,1}^d = \iota(\Delta\delta u_{m,n}) = \frac{u_{m,n}\, \Delta\delta u_{m,n} - \delta u_{m,n}\, \Delta u_{m,n}}{u_{m+1,n}\, u_{m,n}}.$$

These invariants are finite difference approximations of the normalized differential invariants (4.3.19) on a unit square grid in the computational variables. Another possibility is to invariantize the discrete derivatives

$$u_y^{m,n} = \frac{\delta u_{m,n}}{\delta y_n}, \qquad u_{xy}^{m,n} = \frac{\Delta\delta u_{m,n}}{\delta y_n \Delta x_m}, \qquad u_{yy}^{m,n} = \frac{\delta^2 u_{m,n}}{(\delta y_n)^2},$$

to obtain the joint invariants

$$\begin{gathered} I_{0,1}^d = \iota(u_y^{m,n}) = \frac{u_y^{m,n}}{u_{m,n}}, \qquad I_{0,2}^d = \iota(u_{yy}^{m,n}) = \frac{u_{yy}^{m,n}}{u_{m,n}}, \\ I_{1,1}^d = \iota(u_{xy}^{m,n}) = \frac{u_{m+1,n+1}\, u_{m,n} - u_{m+1,n}\, u_{m,n+1}}{u_{m,n}^2\, u_{m+1,n}\, \Delta x_m\, \delta y_n} = \frac{u_{m,n}\, u_{xy}^{m,n} - u_x^{m,n}\, u_y^{m,n}}{u_{m,n}^2\, u_{m+1,n}}. \end{gathered} \tag{4.4.27}$$

In the continuous limit, the invariants (4.4.27) converge to the normalized differential invariants obtained in [**54**].

Our main illustrative pseudo-group (4.2.1) was chosen for its simplicity. This pseudo-group can be embedded into the larger pseudo-group

$$X = f(x), \qquad Y = g(y), \qquad U = \frac{u}{f_x\, g_y}, \qquad f, g \in \mathcal{D}(\mathbb{R}), \tag{4.4.28}$$

which, as observed in the introduction, is the full symmetry group of the differential equation (4.2.3). In the following example, joint invariants of the discretized action (4.4.28) are computed. The results of these computations will be used in Sections 4.5 and 4.6 to construct a fully invariant numerical scheme of equation (4.2.3) and perform numerical tests.

**Example 4.4.20.** The construction of a joint moving frame for the pseudo-group (4.4.28) is similar to the previous example. Though, one important difference between the two examples is that it is no longer possible to work under the assumption that the step size $\delta y_n = k$ is constant as this is not an invariant constraint of the larger pseudo-group (4.4.28). The most one can impose is that the mesh be rectangular

$$\delta x_{m,n} = x_{m,n+1} - x_{m,n} = 0, \qquad \Delta y_{m,n} = y_{m+1,n} - y_{m,n} = 0, \tag{4.4.29}$$

so that $x_{m,n} = x_m$ and $y_{m,n} = y_n$. At the discrete level, the pseudo-group action (4.4.28) can be approximated by the forward discrete action

$$X_m = f_m = f(x_m), \qquad Y_n = g_n = g(y_n), \qquad U_{m,n} = \frac{u_{m,n}}{f_x^m\, g_y^n}, \tag{4.4.30}$$

where

$$f_x^m = \frac{\Delta f_m}{\Delta x_m} = \frac{f_{m+1} - f_m}{x_{m+1} - x_m}, \qquad g_y^n = \frac{\delta g_n}{\delta y_n} = \frac{g_{n+1} - g_n}{y_{n+1} - y_n}.$$

Summarizing the moving frame construction, a cross-section is given by

$$\begin{aligned} \mathcal{K}^{[\infty]}: \qquad x_m = 0, \qquad y_n = 0, \qquad \Delta x_m\, \delta\Delta^2 u_{m,n} - \Delta^2 x_m\, \delta\Delta u_{m,n} = (\Delta x_m)^3\, \delta y_n, \\ u_{m+k,n} = u_{m,n+k} = 1, \qquad k \geq 0, \end{aligned}$$

and the corresponding joint moving frame is

$$\begin{aligned} f_m &= 0, \qquad & f_{m+k} &= \frac{\delta y_n}{g_{n+1}} \sum_{l=0}^{k-1} u_{m+l,n}\, \Delta x_{m+l}, \\ g_n &= 0, \qquad & g_{n+k} &= \frac{g_{n+1}}{u_{m,n} \delta y_n} \sum_{l=0}^{k-1} u_{m,n+l}\, \delta y_{n+l}, \end{aligned} \tag{4.4.31a}$$

where $k \geq 1$, and

$$g_{n+1} = \frac{u_{m,n+1}\, u_{m,n}\, (\Delta x_m)^2\, (\delta y_n)^2}{u_{m+1,n}\, \Delta x_{m+1} \Delta \left[ \dfrac{1}{u_{m,n}\, \Delta x_m} \Delta \left( \dfrac{u_{m,n+1}}{u_{m,n}} \right) \right]}. \tag{4.4.31b}$$

The applications of the invariantization map (4.4.21) to the discrete variables $x_{m+k}$, $y_{n+l}$, $u_{m+k,n+l}$ yields the normalized joint invariants

$$\iota(x_{m+k}) = (\rho^{[\infty]})^* f_{m+k} = \begin{cases} 0 & k = 0, \\ \dfrac{\delta y_n}{g_{n+1}} \displaystyle\sum_{l=0}^{k-1} u_{m+l,n}\, \Delta x_{m+l} & k = 1, 2, 3, \ldots, \end{cases}$$

$$\iota(y_{n+k}) = (\rho^{[\infty]})^* g_{n+k} = \begin{cases} 0 & k = 0, \\ \dfrac{g_{n+1}}{u_{m,n}\delta y_n} \displaystyle\sum_{l=0}^{k-1} u_{m,n+l}\, \delta y_{n+l} & k = 1, 2, 3, 4, \ldots, \end{cases}$$

$$\iota(u_{m+k,n+l}) = \frac{u_{m+k,n+l}}{(\rho^{[\infty]})^* f_x^{m+k}\, (\rho^{[\infty]})^* g_y^{n+k}} = \frac{u_{m+k,n+l}\, u_{m,n}}{u_{m+k,n}\, u_{m,n+k}}, \qquad k, l = 0, 1, 2, \ldots.$$

For later use, the invariantization of

$$u_{xy}^{m,n} = \frac{\delta \Delta u_{m,n}}{\Delta x_m\, \delta y_n}$$

gives the joint invariant

$$I_{1,1}^d = \iota(u_{xy}^{m,n}) = \frac{u_{m+1,n+1}\, u_{m,n} - u_{m+1,n}\, u_{m,n+1}}{u_{m,n}\, u_{m+1,n}\, u_{m,n+1}\, \Delta x_m\, \delta y_n} = \frac{u_{m,n}\, u_{xy}^{m,n} - u_x^{m,n}\, u_y^{m,n}}{u_{m,n}\, u_{m+1,n}\, u_{m,n+1}}. \tag{4.4.32}$$

**Example 4.4.21.** The Lie pseudo-group

$$X = f(x), \qquad Y = e(x, y) = y\, f_x + g(x), \qquad U = u + \frac{e_x}{f_x} = u + \frac{y\, f_{xx} + g_x}{f_x}, \tag{4.4.33}$$

will serve as our last example. This pseudo-group was used by Vessiot in his work on automorphic systems, [**68**]. It is also one of the pseudo-groups used in [**54**] to illustrate the method of equivariant moving frames.

By a similar argument to Example 4.2.1, on a generic mesh $(x_{m,n}, y_{m,n})$, the product pseudo-group action

$$\begin{gathered} X_{m,n} = f(x_{m,n}), \qquad Y = e(x_{m,n}, y_{m,n}) = y_{m,n}\, f_x(x_{m,n}) + g(x_{m,n}), \\ U_{m,n} = u_{m,n} + \frac{e_x(x_{m,n}, y_{m,n})}{f_x(x_{m,n})} \end{gathered} \tag{4.4.34}$$

has no joint invariant since $f(x_{m,n})$, $e(x_{m,n},y_{m,n})$, and $e_x(x_{m,n},y_{m,n})/f_x(x_{m,n})$ are generically independent. To reduce the number of pseudo-group parameters as much as possible, the invariant constraints

$$\delta x_{m,n}=x_{m,n+1}-x_{m,n}=0, \qquad \delta^2 y_{m,n}=y_{m,n+2}-2y_{m,n+1}+y_{m,n}=0 \tag{4.4.35}$$

are imposed. Note that it is not possible to invariantly assume $\Delta y_{m,n}=y_{m+1,n}-y_{m,n}=0$. Hence, rectangular meshes are not invariant for this pseudo-group. Provided $\delta y_{m,n}\neq 0$, which is an invariant constraint of (4.4.34) when (4.4.35) is satisfied, the product pseudo-group action

$$X_m=f(x_m), \quad Y=e(x_m,y_{m,n})=y_{m,n}f_x(x_m)+g(x_m), \quad U_{m,n}=u_{m,n}+\frac{e_x(x_m,y_{m,n})}{f_x(x_m)}$$

admits the joint invariants

$$\frac{y_{m,n+k}-y_{m,n}}{y_{m,n+1}-y_{m,n}}, \qquad u_{m,n+k}-u_{m,n}-\left(\frac{y_{m,n+k}-y_{m,n}}{y_{m,n+1}-y_{m,n}}\right)(u_{m,n+1}-u_{m,n}), \qquad k\in\mathbb{Z}.$$

By the same dilation argument as in Example 4.2.1, it is possible to conclude that these joint invariants cannot approximate all the differential invariants obtained in [**54**]. To construct further joint invariants the product action (4.4.34) is discretized. An admissible discretization is given by

$$\begin{gathered} X_m=f_m=f(x_m), \qquad Y_{m,n}=e_{m,n}=y_{m,n}\,f_x^m+g_m, \\ U_{m,n}=u_{m,n}+\frac{e_x^{m,n}}{f_x^m}=u_{m,n}+\frac{\Delta e_{m,n}}{\Delta f_m}-\frac{\Delta y_{m,n}}{\Delta x_m}=u_{m,n}+\frac{y_{m+1,n}}{\Delta f_m}\Delta\left(\frac{\Delta f_m}{\Delta x_m}\right)+\frac{\Delta g_m}{\Delta f_m}, \end{gathered} \tag{4.4.36}$$

where

$$g_m=g(x_m), \qquad f_x^m=\frac{\Delta f_m}{\Delta x_m} \qquad \text{and} \qquad e_x^{m,n}=\frac{\Delta e_{m,n}}{\Delta x_m}-\frac{\Delta y_{m,n}\,\delta e_{m,n}}{\Delta x_m\,\delta y_{m,n}}.$$

To verify closure of (4.4.36) under composition, let

$$\widetilde{X}_m=\widetilde{f}_m, \qquad \widetilde{Y}_{m,n}=\widetilde{e}_{m,n}=\frac{\Delta\widetilde{f}_m}{\Delta X_m}\,Y_{m,n}+\widetilde{g}_m, \qquad \widetilde{U}_{m,n}=U_{m,n}+\frac{\Delta\widetilde{e}_{mn}}{\Delta\widetilde{f}_m}-\frac{\Delta Y_{mn}}{\Delta X_m}.$$

Thus, in the $x$ variable $\widetilde{X}_m = \widetilde{f}_m = \widetilde{f}(X_m) = \overline{f}_m \circ f_m$, while in the $y$ variable

$$\widetilde{Y}_{mn} = \widetilde{e}_{m,n} = \frac{\Delta \widetilde{f}_m}{\Delta X_m} \left( \frac{\Delta f_m}{\Delta x_m} \, y_{m,n} + g_m \right) + \widetilde{g}_m = \frac{\Delta \widetilde{f}_m}{\Delta x_m} \, y_{m,n} + G_m,$$

with

$$G_m = \frac{\Delta \widetilde{f}_m}{\Delta f_m} \, g_m + \widetilde{g}_m.$$

Finally, in the $u$ variable

$$\begin{aligned} \widetilde{U}_{mn} &= u_{mn} + \frac{\Delta e_{mn}}{\Delta f_m} - \frac{\Delta y_{mn}}{\Delta x_m} + \frac{\Delta \widetilde{e}_{mn}}{\Delta \widetilde{f}_m} - \frac{\Delta Y_{mn}}{\Delta X_m} \\ &= u_{mn} + \frac{\Delta \widetilde{e}_{mn}}{\Delta \widetilde{f}_m} - \frac{\Delta y_{mn}}{\Delta x_m}, \end{aligned}$$

where the equality

$$\frac{\Delta e_{mn}}{\Delta f_m} = \frac{\Delta Y_{mn}}{\Delta X_m}$$

was used.

To obtain a discrete approximation of the moving frame constructed in [**54**], we use the same cross-section replacing derivatives by their finite difference approximations:

$$\begin{gathered} x_{m,n} = y_{m,n} = u_{m,n} = u_x^{m,n} = u_y^{m,n} = u_{xx}^{m,n} = u_{xy}^{m,n} = 0, \\ u_{yy}^{m,n} = 1, \qquad u_{x^{k+3}}^{m,n} = u_{x^{k+2}y}^{m,n} = \cdots = 0, \qquad k \geq 0. \end{gathered}$$

The expressions for the discrete derivatives $u_y^{m,n}$, $u_{yy}^{m,n}$, $u_{yyy}^{m,n}$, and $u_{xyy}^{m,n}$ constraint to (4.4.35) appear in (4.4.12). Solving the normalization equations

$$X_{m,n} = Y_{m,n} = U_{m,n} = U_X^{m,n} = U_Y^{m,n} = U_{XY}^{m,n} = 0, \qquad U_{YY}^{m,n} = 1,$$

we obtain the pseudo-group normalizations

$$f_m = 0, \qquad e_{m,n} = 0, \qquad \frac{\Delta f_m}{\Delta x_m} = \sqrt{u_{yy}^{m,n}}, \qquad \frac{\Delta e_{m,n}}{\Delta x_m} = \sqrt{u_{yy}^{m,n}}\left(\frac{\Delta y_{m,n}}{\Delta x_m} - u_{m,n}\right),$$
$$\frac{\Delta f_{m+1}}{\Delta x_{m+1}} = \sqrt{u_{yy}^{m,n}}\left(1 - \frac{\Delta x_m\, \delta u_{m,n}}{\delta u_{m+1,n}}\right), \qquad \frac{\Delta e_{m+1}}{\Delta x_{m+1}} = \frac{\Delta f_{m+1}}{\Delta x_{m+1}}\left(\frac{\Delta y_{m+1,n}}{\Delta x_{m+1}} - u_{m+1,n}\right),$$
$$\frac{\Delta f_{m+2}}{\Delta x_{m+2}} = \frac{\Delta f_{m+1}}{\Delta x_{m+1}}\left(1 + \frac{\Delta x_{m+1}}{\delta y_{m+2,n}}[\delta y_{m,n}(\Delta y_{m,n} - \Delta x_m\, u_{m,n})u_{yy}^{m,n} - u_{m+1,n+1}]\right).$$

The invariantization map (4.4.21) provides the normalized joint invariants

$$\iota(\Delta x_m) = \Delta x_m \sqrt{u_{yy}^{m,n}}, \qquad \iota(\Delta y_{m,n}) = (\Delta y_{m,n} - u_{m,n}\, \Delta x_m)\sqrt{u_{yy}^{m,n}},$$
$$\iota(\delta y_{m,n}) = \delta y_{m,n} \sqrt{u_{yy}^{m,n}},$$

and

$$I_{03}^d = \iota(u_{yyy}^{m,n}) = \frac{u_{yyy}^{m,n}}{(u_{yy}^{m,n})^{3/2}}, \qquad I_{1,2}^d = \iota(u_{xyy}^{m,n}) = \frac{u_{xyy}^{m,n} + u_{m,n}\, u_{yyy}^{m,n} + 2u_y^{m,n}\, u_{yy}^{m,n}}{(u_{yy}^{m,n})^{3/2}}. \tag{4.4.37}$$

In the continuous limit, the joint invariants (4.4.37) converge to the differential invariants

$$I_{0,3}^d \to I_{0,3} = \frac{u_{yyy}}{u_{yy}^{3/2}}, \qquad I_{1,2}^d \to I_{1,2} = \frac{u_{xyy} + u\, u_{yyy} + 2u_y\, u_{yy}}{u_{yy}^{3/2}},$$

as obtained in [**54**].

## 4.5. Differential and finite difference equations

This section recalls basic definitions pertaining to invariant differential equations and their invariant finite difference approximations, [**40, 48**]. To treat differential equations and finite difference equations on a similar footing, computational variables are introduced in the continuous setting. Given a differential equation

$$\Delta(x, u^{(n)}) = 0, \tag{4.5.1}$$

the chain rule (4.3.10) may be used to re-express (4.5.1) in terms of $x^i = x^i(s)$, $u^\alpha = u^\alpha(s)$ and their computational derivatives $x^i_{s^A}$, $u^\alpha_{s^A}$:

$$\overline{\Delta}(s, x^{(n)}, u^{(n)}) = \Delta(x, u^{(n)}) = 0, \tag{4.5.2a}$$

where $(x^{(n)}, u^{(n)}) = (\ldots\ x^i_{s^A}\ \ldots\ u^\alpha_{s^A}\ \ldots)$ on the left-hand side of (4.5.2a) and $u^{(n)} = (\ldots\ u^\alpha_{x^J}\ \ldots)$ on the right-hand side. Equation (4.5.2a) can be supplemented by *companion equations*, [**46**],

$$\widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0, \tag{4.5.2b}$$

which impose restrictions on the change of variables $s \mapsto x(s)$. For the *extended system* (4.5.2) to have the same solution space as the original equation (4.5.1), the companion equations (4.5.2b) cannot introduce differential constraints on the derivatives $u^\alpha_{s^A}$. Also, they must respect the non-degeneracy condition (4.3.8).

**Definition 4.5.1.** A Lie pseudo-group $\mathcal{G}$ is said to be a *symmetry (pseudo-)group* of a differential equation $\Delta(x, u^{(n)}) = 0$ if for $g \in \mathcal{G}$,

$$\Delta(g \cdot x, g^{(n)} \cdot u^{(n)}) = 0 \qquad \text{whenever} \qquad \Delta(x, u^{(n)}) = 0.$$

An extended system of differential equations $\{\overline{\Delta}(s, x^{(n)}, u^{(n)}) = 0,\ \widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0\}$ is $\mathcal{G}$-*compatible* with the $\mathcal{G}$-invariant differential equation $\Delta(x, u^{(n)}) = 0$ if it is invariant under the pseudo-group $\mathcal{G}$:

$$\begin{cases} \overline{\Delta}(s, g^{(n)} \cdot x^{(n)}, g^{(n)} \cdot u^{(n)}) = 0, \\ \widetilde{\Delta}(s, g^{(n)} \cdot x^{(n)}, g^{(n)} \cdot u^{(n)}) = 0, \end{cases} \qquad \text{whenever} \qquad \begin{cases} \overline{\Delta}(s, x^{(n)}, u^{(n)}) = 0, \\ \widetilde{\Delta}(s, x^{(n)}, u^{(n)}) = 0. \end{cases}$$

Using a perspective slightly different from the one introduced in [**8, 40**], a numerical scheme for the differential equation (4.5.1), or its extended counterpart (4.5.2), is a set of finite difference equations

$$E(\mathfrak{z}_N^{[n]}) = 0, \qquad \widetilde{E}(\mathfrak{z}_N^{[n]}) = 0,$$

having the property that, in the continuous limit, these equations converge to the extended system (4.5.2):

$$E(\mathfrak{z}_N^{[n]}) \to \overline{\Delta}(s, x^{(n)}, u^{(n)}), \qquad \widetilde{E}(\mathfrak{z}_N^{[n]}) \to \widetilde{\Delta}(s, x^{(n)}, u^{(n)}). \tag{4.5.3}$$

**Definition 4.5.2.** A discretized pseudo-group $\mathcal{G}_d$ is a *symmetry group* of the numerical scheme $\{E(\mathfrak{z}_N^{[n]}) = 0,\, \widetilde{E}(\mathfrak{z}^{[n]}) = 0\}$ if

$$\begin{cases} E(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}) = 0, \\ \widetilde{E}(g_N^{[n]} \cdot \mathfrak{z}_N^{[n]}) = 0, \end{cases} \qquad \text{whenever} \qquad \begin{cases} E(\mathfrak{z}_N^{[n]}) = 0, \\ \widetilde{E}(\mathfrak{z}_N^{[n]}) = 0. \end{cases}$$

Given a $\mathcal{G}$-invariant differential equation $\Delta = 0$, there are many different strategies for constructing an invariant numerical scheme, [**2, 33, 40, 50, 63**]. Assuming $\Delta$ is a differential invariant, one possibility is to obtain an invariant discretization $E$ of $\Delta$ using moving frames. This can be done algorithmically by first discretizing $\Delta$ to obtain a finite difference approximation $F$. Since this discretization is not necessarily invariant, see Example 4.5.3 for an illustration of this fact, an invariant discretization of $\Delta$ is obtained by invariantizing $F$:

$$\Delta \sim E = \iota(F).$$

An invariant approximation of $\Delta = 0$ is then given by $E = 0$. As for the mesh equations $\widetilde{E} = 0$, there is, unfortunately, no clear algorithm for determining these equations. Nevertheless, there are obvious requirements that need to be satisfied. First, these equations must include the invariant constraints occurring in the construction of a joint moving frame for the discretized pseudo-group action $\mathcal{G}_d$. For example, in Example 4.4.19, the invariant constraint permitting the construction of a joint moving frame is given by

$$x_{m,n+1} - x_{m,n} = 0, \tag{4.5.4}$$

and this equation would need to be part of the mesh equations of any invariant numerical scheme constructed from the joint moving frame (4.4.25). For some pseudo-group actions it might be possible to add further invariant mesh equations provided the non-degeneracy constraint (4.4.4) is satisfied. For example, in Example 4.4.19, since $Y_{m,n} = y_{m,n}$ is invariant, we assumed that $y_n = k\,n + y_0$ to simplify computations. Under this assumption, equation (4.5.4) would be supplemented by the invariant mesh equations

$$y_{m+1,n} - y_{m,n} = 0, \qquad y_{m,n+1} - y_{m,n} = k.$$

**Example 4.5.3.** A numerical scheme for the differential equation (4.2.3) invariant under the full (discretized) symmetry pseudo-group (4.4.30) is constructed. Following the prescription above, the invariant (4.2.2) is naively discretized on a rectangular mesh

$$I_{1,1} \sim F = \frac{u_{m+1,n+1}\,u_{m,n} - u_{m+1,n}\,u_{m,n+1}}{u_{m,n}^3\,\Delta x_m\,\delta y_n}. \tag{4.5.5}$$

We note that this approximation is not invariant under (4.4.30). Using the results of Example 4.4.20, an invariant approximation is obtained by invariantizing (4.5.5):

$$I_{1,1} \sim I_{1,1}^d = \iota(F) = \frac{u_{m+1,n+1}\,u_{m,n} - u_{m+1,n}\,u_{m,n+1}}{u_{m,n}\,u_{m+1,n}\,u_{m,n+1}\,\Delta x_m\,\delta y_n}.$$

The construction of the joint moving frame in Example 4.4.20 is based on the assumption that (4.4.29) holds. Hence, an invariant numerical scheme for (4.2.3) is given by

$$\frac{u_{m+1,n+1}\,u_{m,n} - u_{m+1,n}\,u_{m,n+1}}{u_{m,n}\,u_{m+1,n}\,u_{m,n+1}\,\Delta x_m\,\delta y_n} = 1, \tag{4.5.6a}$$

with mesh equations

$$\delta x_{m,n} = 0, \qquad \Delta y_{m,n} = 0. \tag{4.5.6b}$$

The scheme (4.5.6) is an approximation of the differential equations

$$I_{1,1} = \frac{u\,u_{st} - u_s\,u_t}{u^3\,x_s\,y_t} = 1 \tag{4.5.7a}$$

and

$$x_t = 0, \qquad y_s = 0, \tag{4.5.7b}$$

in the computational variables $x = x(s,t)$, $y = y(s,t)$, $u = u(s,t)$. Equation (4.5.7a) is simply (4.2.3) expressed in computational variables while equations (4.5.7b) are the invariant companion equations of the extended system (4.5.7).

## 4.6. Numerical simulations

In this section, the fully invariant numerical scheme (4.5.6) is compared with the standard finite difference approximation

$$\begin{gathered} \frac{u_{m+1,n+1}\, u_{m,n} - u_{m+1,n}\, u_{m,n+1}}{u_{m,n}^3\, \Delta x_m\, \delta y_n} = 1, \\ \Delta x_{m,n} = h, \qquad \delta x_{m,n} = 0, \qquad \Delta y_{m,n} = 0, \qquad \delta y_{m,n} = k \end{gathered} \tag{4.6.1}$$

of equation (4.2.3). Since the mesh equations (4.5.6b) do not specify the step sizes $\Delta x_{m,n}$ and $\delta y_{m,n}$, the equations

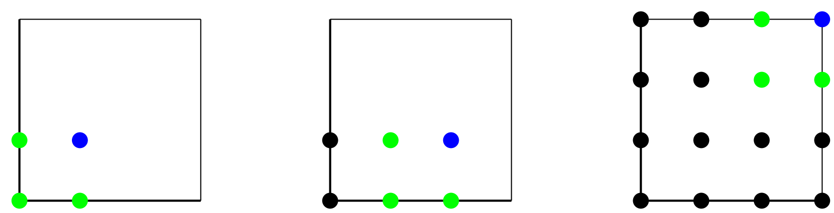
$$\Delta x_{m,n} = h, \qquad \delta y_{m,n} = k$$

are supplemented to compare the two schemes on the same footing. In other words, the numerical schemes (4.5.6a) and (4.6.1) are both defined over the same rectangular mesh.

### 4.6.1. Methodology

Equations (4.6.1) and (4.5.6a) both relate the values of the solution $u$ at the four corners of a rectangle on the mesh. Given, the value of $u$ at three corners, the equations provide the value of $u$ at the remaining vertex. These equations are suited for initial value problems (IVPs). For example, the value of $u$ in the $xy$-plane can be calculated if initial conditions on $u$ are specified on two perpendicular axes.

Though, in practice, one has to limit itself to a finite rectangular domain and the specification of $u$ on two of its sides will completely determine the solution on the rectangle. Figure 4.4 illustrates the situation on a $4 \times 4$ rectangle. At each step the value of $u$ at the blue dot is a function of the solution at the green dots. Filling the rectangle from left to right and then from bottom up, the whole rectangle is covered.



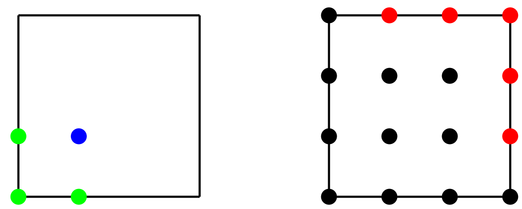
(a) 1st step. (b) 2nd step. (c) 9th step.

FIG. 4.4. Initial value problem on a rectangle.

On the other hand, numerical schemes like (4.6.1) and (4.5.6a) are ill-defined for boundary value problems (BVP) on rectangular domains. Figure 4.5 illustrates the issue. If, for example, one starts the iterative process in the bottom left corner of the domain of integration, then all points on the right and top boundaries highlighted in red in Figure 4.5(b) are ill-defined since their values are simultaneously specified by the boundary conditions and the numerical scheme.

Since in Section 4.6.2 we are interested in solving BVPs numerically, we now explain how to adapt the schemes (4.6.1) and (4.5.6a) to BVPs on rectangular domains. For this, we note that each point in the interior domain can be computed in four different ways using the numerical schemes. First, solving for $u_{m+1,n+1}$ in the invariant scheme (4.5.6) we obtain

$$u_{m+1,n+1} = u_{m+1,n}\, u_{m,n+1} \left( \frac{1}{u_{m,n}} + h\, k \right). \tag{4.6.2}$$



(a) Bottom left corner start.

(b) End result.

FIG. 4.5. Ill-defined boundary value problem on a rectangle.

Then, shifting (4.5.6) from $(m, n)$ to $(m + 1, n)$, the solution $u_{m+1,n+1}$ can also be expressed as

$$u_{m+1,n+1} = \frac{u_{m+1,n}\, u_{m+2,n+1}}{u_{m+2,n}(1 + h\, k\, u_{m+1,n})}. \tag{4.6.3}$$

Similarly, shifting the invariant scheme (4.5.6) from $(m, n)$ to $(m, n + 1)$ and $(m + 1, n + 1)$ we obtain

$$u_{m+1,n+1} = \frac{u_{m,n+1}\, u_{m+1,n+2}}{u_{m,n+2}(1 + h\, k\, u_{m,n+1})}, \qquad u_{m+1,n+1} = \frac{u_{m+1,n}\, u_{m+2,n+1}}{u_{m+2,n}(1 + h\, k\, u_{m+1,n})}. \tag{4.6.4}$$

Defining $u_{m+1,n+1}$ to be the average of the four equations (4.6.2), (4.6.3), (4.6.4) yields a finite difference equation expressing each interior point in the domain as a function of its eight surrounding points as illustrated in Figure 4.6. The same procedure applies to the standard scheme (4.6.1). The two new schemes are now well-adapted to BVPs on rectangular domains since there is no conflict between the points computed using the numerical schemes and the boundary conditions.

Solutions to BVPs are then obtained by applying the *relaxation method*. The first step in the implementation of the relaxation method consists of assigning values to the points inside the domain of integration. In principle, arbitrary values can be assigned but it is always advantageous to assign well-educated initial values. In our

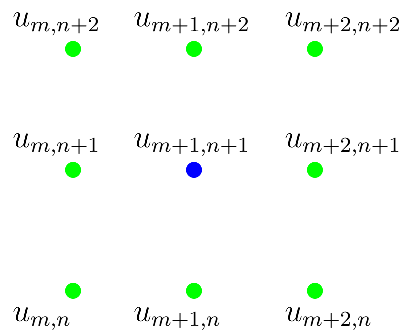
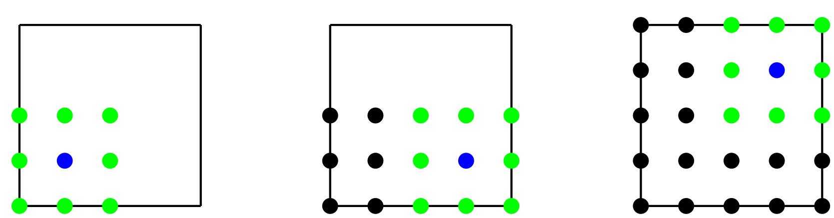



FIG. 4.6. New scheme on nine points. The value of $u$ at the blue dot is determined by the neighbouring green points.

case, we decided to use the average of the four solutions obtained by solving the IVPs starting in each corner of the rectangular domain. Once this is done, new values are assigned to the interior points using the BVP adapted scheme. Figure 4.7 illustrates the order in which one could assign these new interior values on a $5 \times 5$ square. Recomputing the interior values once using the most recent data is one iteration of the relaxation process. If the scheme is stable, by iterating the relaxation process the interior values will converge towards the scheme's solution.



(a) 1st step. (b) 3rd step. (c) 9th step.

FIG. 4.7. Scheme on nine points covering a rectangular BVP.

### 4.6.2. Numerical results and analysis

Three BVPs were tested using the exact solutions

$$u = \frac{2}{(x+y)^2}, \qquad u = 2\sec^2(x+y), \qquad u = \frac{2e^{x+y}}{(e^{x+y}-1)^2}, \tag{4.6.5}$$

obtained in [**59**]. In each case, the boundary condition is given by the value of the exact solution on the edges of a rectangular domain. We note that the first and third solutions are not defined along the line $y + x = 0$ and diverge to infinity on both sides of the singular line. The second solution also diverges along the lines $y + x = \pi/2 + n\pi$, with $n \in \mathbb{Z}$. Since the quantitative results are similar for each solution, only the secant solution is presented below.

Table 4.1 lists the average error of the invariant and standard schemes (4.5.6) and (4.6.1) for different values of $h$ and $k$ for the secant solution on the unit square $[1,2]\times[1,2]$ after 100 iterations of the relaxation procedure. For the cases considered, the invariant scheme is roughly three times more precise than the standard scheme.

| Scheme | $h,k = 0.1$ | $h,k = 0.05$ | $h,k = 0.01$ | $h,k = 0.005$ |
|---|---|---|---|---|
| Standard | $2.19 \times 10^{-1}$ | $1.07 \times 10^{-1}$ | $3.23 \times 10^{-2}$ | $1.66 \times 10^{-2}$ |
| Invariant | $4.12 \times 10^{-2}$ | $2.75 \times 10^{-2}$ | $1.03 \times 10^{-2}$ | $5.42 \times 10^{-3}$ |

TAB. 4.1. Average errors on $[1,2]\times[1,2]$ for the secant solution after 100 relaxation iterations.

As demonstrated in [**8, 33**], invariant schemes seem to shine near singularities. Here again the invariant scheme is more precise and stable near singularities. Table 4.2 shows the maximal error for both methods when the bottom left corner of the unit square of integration is brought closer to the exact solution singularity at $(\pi/4, \pi/4) \approx (0.785, 0.785)$. The first row in the table gives the coordinates $(x_0, y_0)$

of the square of integration's bottom left corner. The step size in the independent variables is set to $h = k = 0.01$, and the relaxation process was again run a hundred times. As the square of integration gets closer to the singularity, Table 4.2 shows that the precision of the standard method gets worst much faster than the invariant scheme. Moreover, when $x_0 = y_0 = 0.84$ or anywhere closer to the singularity $(\pi/4, \pi/4)$, the standard scheme becomes unstable while the invariant method integrates further into the singularity. As shown in Figure 4.8(b), while the source of the instability is in the bottom left corner, its manifestation appears first in the opposite corner for the standard method. Meanwhile, the invariant method, Figure 4.8(c), is faithful to the exact solution, Figure 4.8(a).

| Scheme | $x_0 = y_0 = 0.87$ | 0.86 | 0.85 | 0.84 |
|---|---|---|---|---|
| Standard | 2.20 | 4.92 | 129.03 | unstable |
| Invariant | $3.12 \times 10^{-1}$ | $4.46 \times 10^{-1}$ | $6.78 \times 10^{-1}$ | 1.15 |

TAB. 4.2. Maximal errors on a unit square near the singularity $(\pi/4, \pi/4)$.

It is not difficult to understand why the invariant scheme produces better results when compared to the standard scheme. The distinctive feature between the two schemes is the way the cubic term $u^3$ in (4.2.3) is approximated. In the naive discretization (4.6.1), $u^3$ is approximated by the nonlinear term $u_{m,n}^3$. This cubic term in the standard scheme requires the use of a nonlinear equation solver like Newton's method at each iteration of the relaxation method which increases the computational cost and adds instability. On the other hand, in the invariant scheme the cubic term $u^3$ is approximated by $u_{m,n}\, u_{m+1,n}\, u_{m,n+1}$. By using the values of $u$ at three distinct points, the invariant method is more precise and stable, especially where the solution varies a lot. Moreover, (4.5.6) can be solved for any of the $u$'s without the need to resort to a nonlinear solver. Thanks to this simplification, the computation time for the invariant method was approximately three times shorter than that of the standard method in all our numerical simulations.

As previously mentioned, similar results were also obtained for the rational and exponential solutions of (4.6.5).

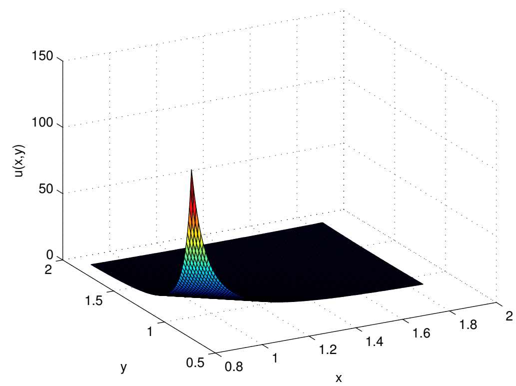
## 4.7. Conclusion

To the best of our knowledge, this is the first work attempting to construct invariant numerical schemes of differential equations with infinite-dimensional symmetry groups. As our examples show, the main issue with considering the product action of Lie pseudo-groups is the shortage of joint invariants to approximate differential invariants. To circumvent this problem, we proposed to discretize the action by replacing derivatives with finite difference approximations. To illustrate our constructions as clearly as possible, we chose simple Lie pseudo-group actions that have been well studied in the continuous setting. The next natural step in this line of research would be to consider more substantial symmetry pseudo-groups and apply Lie theoretical tools to these invariant schemes to find explicit solutions.

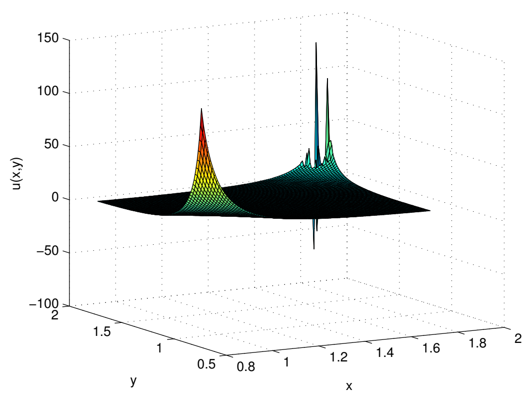
The main emphasis of the paper was on the theoretical aspects that emerge when infinite-dimensional symmetry groups are discretized. Although the numerical simulations performed in Section 4.6 do not have the pretension to be the state of the art in numerical analysis, they indicate that invariant schemes can produce good numerical results. It remains a challenge to bridge the gap between the most recent trends in numerical analysis and the latest developments in the theory of invariant finite difference equations.

## Acknowledgement

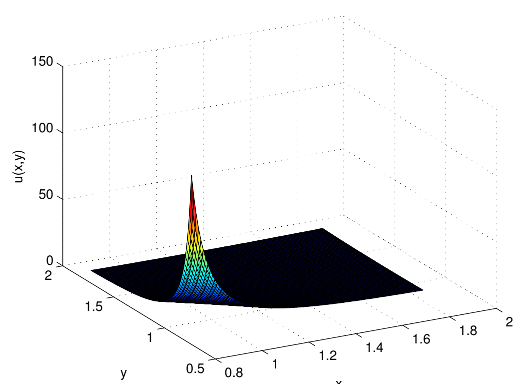
We thank Alexander Bihlo for stimulating discussions on the project, and Pavel Winternitz for his comments on the manuscript. The research of Raphaël Rebelo was supported in part by an FQRNT Doctoral Research Scholarship while the research of Francis Valiquette was supported in part by an AARMS Postdoctoral Fellowship.




(a) Exact solution.




(b) Standard scheme.




(c) Invariant scheme.

FIG. 4.8. Secant solution near the singularity $(\pi/4, \pi/4)$.

# Chapter 5

## CONCLUDING REMARKS AND FUTURE RESEARCH

The use of computational variables has provided a simple and straightforward method for introducing discrete partial derivatives on arbitrary meshes. By construction, these discrete derivatives always converge toward their continuous counterparts even after having been acted upon by a group transformation in the neighborhood of the identity. This feature has theoretical and practical consequences. From a practical point of view, it facilitates invariant discretization since it is possible to pick the "same" cross-section in the continuous and discrete cases and it guarantees that the discrete invariants converge to the continuous ones. Before, when a complete set of invariants had been computed in the discrete and the continuous, the continuous limit of the discrete set was not converging, in general, to the continuous set, but to some functions of the continuous invariants. It then took cumbersome calculations to construct discrete invariants that converge to the continuous objects that were being approximated. The fact that the continuous limits are now automatically given by the method is a consequence of the more fundamental fact that those discrete derivatives make it possible to write a discrete jet space that corresponds to the continuous jet space term by term. Many continuous objects of Lie's theory can be reexpressed in this discrete setting. For example, a discrete prolongation of the action which goes, term by term, to the continuous prolongation of the group action can be written.

As indicated at the end of Chapter 3, once an invariant discretization method for PDEs invariant under Lie groups is obtained, it seems natural to extend the method to PDEs invariant under Lie pseudo-groups. We have been able to do this by creating a new object called a discretized pseudo-group. Chapter 4 laid down the foundations for this new object and applied it to some examples. A numerical algorithm was also proposed to adapt typical finite difference schemes to boundary value problems. All invariant discretizations presented in this thesis proved to be more precise than standard finite difference schemes. They were also more stable near singularities. We do not claim to be comparing symmetry preserving discretization with the most powerful methods existing in numerical analysis. However, our results indicate that invariant schemes present advantages over standard finite difference methods.

It would be interesting to further refine invariant numerical methods. The invariant schemes proposed in this thesis (and in most articles published in the field) are typically one-step explicit schemes, invariant counterparts of standard finite difference schemes. Copying the evolution of numerical techniques, it would be easy to create more evolved invariant schemes: implicit, predictor-corrector, and so on. One could even try to recast finite elements methods in terms of invariants. In all cases, a bridge should be built between popular techniques in numerical analysis and invariant methods. The recent work of Bihlo is an inspiring step in that direction, [**3**]. The implementation of the method into computer software would also be useful.

Although the basics of discretized pseudo-groups were laid down in this thesis, many questions remain unanswered. For example, it would be interesting to determine the effects of the choice made when discretizing the group action, see Example **??**, and, more specifically, how this choice affects the algebraic expressions and the errors and stability of the schemes.

Finally, despite some recent progress, symmetry reduction is still the Achilles heel of Lie's theory applied to discrete equations. However, computational variables might bring a new perspective to help solve this problem. A big difference between differential equations and their corresponding invariant schemes is that the schemes are systems of equations relying on new variables hidden in the indices. As such, the structure of the discrete schemes is more similar to the one of extended systems. Recall that extended systems are differential equations expressed in computational variables (**??**) with companion equations (**??**) determining the relation between computational variables and hold independent variables. The following simple example illustrates how the knowledge of enough symmetries makes possible the complete reduction of invariant schemes to system of algebraic equations on one point.

**Example 5.0.1.** Consider the second order ODE

$$u'' = F(u'), \tag{5.0.1}$$

where $F$ is an arbitrary function. The symmetry group of (5.0.1) is

$$X = x + \epsilon_1, \qquad U = u + \epsilon_2, \tag{5.0.2}$$

for arbitrary $F(z)$; for specific functions $F(z)$, it may be larger. The two-dimensional abelian group (5.0.2) makes possible to solve (5.0.1) by quadrature using standard techniques, [**48**]. An extended system for (5.0.1) is

$$u_{ss} = F(u_s), \qquad x_s = 1. \tag{5.0.3}$$

It is a system of one second order equation and a first order one. An invariant scheme for (5.0.1) is given by

$$u^i_{xx} = F(u^i_x), \qquad \Delta x_i = h, \tag{5.0.4}$$

where $h$ is a constant and

$$u^i_x = \frac{\Delta u_i}{\Delta x_i}, \qquad u^i_{xx} = \frac{\Delta^2 u_i}{(\Delta x_i)^2}.$$

It is a system of one equation on three points and one equation on two points. For both the extended system (5.0.3) and the invariant scheme (5.0.4), the two-dimensional symmetry group (5.0.2) is insufficient to completely reduce the systems. By completely reduced I mean reduced to a system of algebraic equations on one point. However, if group action on the computational variables is allowed, the extended system (5.0.3) is invariant under the *extended group*

$$S = s + \epsilon_0, \qquad X = x + \epsilon_1, \qquad U = u + \epsilon_2, \tag{5.0.5}$$

which can be used to apply reduction as follows. Translational invariance in $x$ and $u$ invokes the change of variables $z = u_s$ and $\zeta = x_s$. System (5.0.3) then becomes

$$z_s = F(z), \qquad \zeta = 1. \tag{5.0.6}$$

On the other hand, invariance under translations of $s$ invokes the change of variables

$$y = z, \qquad v = s.$$

The system (5.0.6) then becomes

$$k = \frac{1}{F(y)}, \qquad \zeta = 1, \tag{5.0.7}$$

with $k = v_y$. Similarly in the discrete case, invariance under translations in $u$ and $x$ prompts the change of variables $z_i = u_x^i$ and $\zeta_i = \Delta x_i$. The system (5.0.4) becomes

$$z_x^i = F(z_i), \qquad \zeta_i = h. \tag{5.0.8}$$

It is now possible to mimick the invariance under translations of the index variable $s$ in the continuous, by setting

$$y_i = z_i, \qquad v_i = s_i.$$

This implies that $\Delta v_i = \Delta s_i = 1$. The system (5.0.8) then becomes

$$k_i = \frac{1}{h\,F(y_i)}, \qquad \zeta_i = h, \tag{5.0.9}$$

with $k_i = \dfrac{\Delta v_i}{\Delta y_i}$. In the continuous limit, the reduced discrete scheme (5.0.9) converges to the reduced continuous equation (5.0.6).

Although the previous reduction poses a certain number of theoretical questions, it is a path to symmetry reduction which seems worth exploring.

Since this thesis was devoted to the development of Lie's theory applied to partial difference equations (P$\Delta$E) and since the theory applied to ordinary difference equations (O$\Delta$E) is in a much more mature state, it is pertinent to close this dissertation with a comparison of those two paradigms. For ODEs, infinite dimensional symmetries only arise for equations of the first order (two points) and the knowledge of a one dimensional subgroup is sufficient to generate the general solution. In this case, the invariant difference schemes can be so chosen that their solutions coincide exactly with those of the original differential equation, [**65**]. Thus, numerical methods are useful when there is not enough symmetries to completely reduce the system or when the reduction leads to transcendental equations, [**7**]. The situation is more complex for PDEs. Although the knowledge of symmetries enables to generate particular invariant solutions, [**48**], most nonlinear equations can only be solved numerically. This thesis and many articles cited in it tend to show that it is beneficial to use invariant difference schemes when looking for numerical solutions of PDEs. When a given PDE is invariant under a pseudo-group we propose to discretize this pseudo-group in order to obtain an invariant scheme. This process transforms the continuous point transformations into generalized transformations in the discrete space. Finally, symmetry reduction for P$\Delta$Es is even less understood than for ordinary difference equations and is definitely a question to explore in the coming years. Dorodnitsyn skims through the subject in his recent book, [**22**]. Using Dorodnitsyn ideas, it seems possible to apply the logic presented in Example 5.0.1 to reduce P$\Delta$Es. While in Example 5.0.1, each one dimensional symmetry leads to the disappearance of one variable evaluated at one point, thus reducing the order, in the P$\Delta$Es case, a one dimensional symmetry leads to the disappearance of one variable. Since in the computational variables approach, the indices are variables in their own right, it should be possible to use symmetries to decrease the number of indices. In some cases, it might even be possible to reduce to a single independent variable and obtain particular solutions of P$\Delta$Es by solving O$\Delta$Es.

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